Document made available under the Patent Cooperation Treaty (PCT)

International application number: PCT/US05/001338

International filing date:

13 January 2005 (13.01.2005)

Document type:

Certified copy of priority document

Document details:

Country/Office: US

Number:

60/536,451

Filing date:

13 January 2004 (13.01.2004)

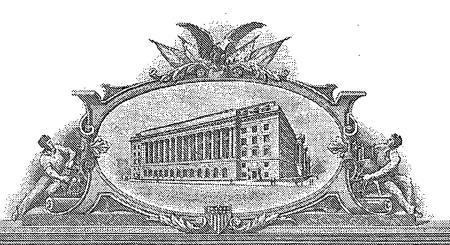
Date of receipt at the International Bureau: 03 March 2005 (03.03.2005)

Remark:

Priority document submitted or transmitted to the International Bureau in

compliance with Rule 17.1(a) or (b)





AND BURGER OF THE CONTRACT OF THE PROPERTY OF

and and and vindou and sit preserves seam (doug):

UNITED STATES DEPARTMENT OF COMMERCE

United States Patent and Trademark Office

February 18, 2005

THIS IS TO CERTIFY THAT ANNEXED HERETO IS A TRUE COPY FROM THE RECORDS OF THE UNITED STATES PATENT AND TRADEMARK OFFICE OF THOSE PAPERS OF THE BELOW IDENTIFIED PATENT APPLICATION THAT MET THE REQUIREMENTS TO BE GRANTED A FILING DATE.

APPLICATION NUMBER: 60/536,451 FILING DATE: January 13, 2004

RELATED PCT APPLICATION NUMBER: PCT/US05/01338

Certified by

Under Secretary of Commerce for Intellectual Property and Director of the United States Patent and Trademark Office



1287275

_
සු
တ္ပ
~
_
_

PTO/SB/16 (08-03)

Approved for use through 07/31/2006. OMB 0651-0032
U.S. Patent and Trademark Office; U.S. DEPARTMENT OF COMMERCE

Under the Paperwork Reduction Act of 1995, no persons are required to respond to a collection of information unless it displays a valid OMB control number.

PROVISIONAL APPLICATION FOR PATENT COVER SHEET

This is a request for filing a PROVISIONAL APPLICATION FOR PATENT under 37 CFR 1.53(c).

Express Mail Label No. EU604545486US

D .	INVENTOR	R(S)					
Given Name (first and middle (if any))				ountry)			
Scott C.	Garman		Rockville	, MD		٠ <u>٠</u>	
Additional inventors are being named on the	1	separately num	bered sheets a	ttached h	ereto	مَنْ	
TITLE OF THE INVENTION (500 characters max)							
CRYSTAL STRUCTURE OF HUMAN ALPHA-GALACTOSIDASE						154 U.S	
Direct all correspondence to: CO	RRESPONDENCE ADDRESS	$\overline{}$				0/5	
Customer Number:						25. 6	
OR							
Firm or Individual Name Konstantinos Andrikopoulos, JD, PhD							
Address Transkaryotic Therapies, Inc.							
Address 700 Main St.	······································						
City Cambridge		State	МА	Zip	02139		
Country U.S.A.		Telephone	(617) 613-4255	Fax	(617) 613-4494		
ENCLOSED APPLICATION PARTS (check all that apply)							
Specification Number of Pages 39 CD(s), Number							
✓ Drawing(s) Number of Sheets 91		V	Other (specify) Sequence Listing 3pg				
Application Date Sheet. See 37 CFR 1.76							
METHOD OF PAYMENT OF FILING FEES FOR THIS PROVISIONAL APPLICATION FOR PATENT							
Applicant claims small entity status. See 37 CFR 1.27. FILING FEE							
Amount (\$) A check or money order is enclosed to cover the filing fees.							
The Director is herby authorized to charge filling fees or credit any overpayment to Deposit Account Number: 502647							
Payment by credit card. Form PTO-2038 is attached.							
The invention was made by an agency of the United States Government or under a contract with an agency of the United States Government. No. Yes, the name of the U.S. Government agency and the Government contract number are: NIAID, NIH							
[Page 1 of 2] Respectfully submitted.			Date_January 13, 2004				
SIGNATURE Komstantinos Andrikogonlos			REGISTRATION NO. 48,915				
TYPED or PRINTED NAME Konstantinos Andrikopoulos (if appropriate) Odoset Number: 0402							

TELEPHONE (617) 613-4255

USE ONLY FOR FILING A PROVISIONAL APPLICATION FOR PATENT

USE ONLY FOR FILING A PROVISIONAL APPLICATION FOR PATENT
This collection of information is required by 37 CFR 1.51. The information is required to obtain or retain a benefit by the public which is to file (and by the USPTO to process) an application. Confidentiality is governed by 35 U.S.C. 122 and 37 CFR 1.14. This collection is estimated to take 8 hours to complete, including gathering, preparing, and submitting the completed application form to the USPTO. Time will vary depending upon the individual case. Any comments on the amount of time you require to complete this form and/or suggestions for reducing this burden, should be sent to the Chief Information Officer, U.S. Patent and Trademark Office, U.S. Department of Commerce, P.O. Box 1450, Alexandria, VA 22313-1450. DO NOT SEND FEES OR COMPLETED FORMS TO THIS ADDRESS. SEND TO: Mail Stop Provisional Application, Commissioner for Patents, P.O. Box 1450, Alexandria, VA 22313-1450.

PROVISIONAL APPLICATION COVER SHEET Additional Page

PTO/SB/16 (08-03)

Approved for use through 07/31/2006. OMB 0651-0032

U.S. Patent and Trademark Office, U.S. DEPARTMENT OF COMMERCE

Under the Paperwork Reduction Act of 1995, no persons are required to respond to a collection of information unless it displays a valid OMB control number.

Docket Number 0402

	0402		
	INVENTOR(S)/APPLICANT(S)		
Given Name (first and middle [if any])	Family or Surname	Residence (City and either State or Foreign Country)	
David N.	Garboczi	Gaithersburg,-MD	
Richard F.	Selden	Wellesley, MA	
Douglas A.	Treco	Arlington, MA	
Michael W.	Heartlein	Boxborough, MA	
Marianne	Borowski	Glen, NH	
	·	,	
·			
	·		

[Page 2 of 2]

CRYSTAL STRUCTURE OF HUMAN α-GALACTOSIDASE

5

20

Field of the Invention

This invention relates to the X-ray crystal structure of the human α -galactosidase glycoprotein. More specifically, the invention relates to crystallized compositions of human α -galactosidase and to crystallized complexes of human α -galactosidase and its catalytic product α -galactose. The invention further relates to a computer programmed with the structure coordinates of the human α -galactosidase's active site wherein said computer is capable of displaying a three-dimensional representation of that active site. The invention also relates to methods for rational drug design based on the structural data for human α -galactosidase provided on computer readable media, as analyzed on a computer system having suitable computer algorithms.

Background of the Invention

The lysosomal enzyme α-galactosidase (α-GAL or α-Gal A, E.C. 3.2.1.22, SEQ ID NO:2) 'catalyzes the removal of galactose from oligosaccharides, glycoproteins, and glycolipids during the catabolism of macromolecules (FIG. 5a). Deficiencies in lysosomal enzymes lead to the accumulation of substrates in the tissues, conditions known as lysosomal storage diseases. In humans, the absence of functional α-GAL leads to the accumulation of galactosylated substrates (primarily globotriaosylceramide, FIG. 5b) in the tissues, leading to Fabry disease, an X-linked recessive disorder first described in 1898 (Fabry, J. Arch. Dermatol. Syph., 1898, 43:187) characterized by chronic pain, ocular opacities, liver and kidney impairment, skin lesions, vascular deterioration and/or cardiac deficiencies (Brady, R. O., et al., N. Engl. J. Med., 1967, 276:1163-7; Desnick, R. J., et al., In The Metabolic and Molecular Bases of Inherited Disease 8th edit. -Scriver, C. R., Beaudet, A. L., Sly, W. S. & Valle, D., eds.-, 2001, pp. 3733-3774. McGraw-Hill, New York). Recombinant human α-GAL has the ability to restore enzyme function in patients (Schiffmann, R., et al., JAMA, 2001, 285:2743-9; Eng, C. M., et al., N. Engl. J. Med., 2001, 345:9-16), and enzyme replacement therapy using α-GAL was recently approved in the United States as a treatment for Fabry disease. α-GAL became the second recombinant protein approved for the treatment of a lysosomal storage disorder (after \beta-glucosidase, a treatment for Gaucher disease - Beutler, E. & Grabowski, G. A., 2001, Gaucher Disease. In *The Metabolic and Molecular Bases of Inherited Disease* 8th edit. -Scriver, C. R., Beaudet, A. L., Sly, W. S. & Valle, D., eds.-McGraw-Hill, New York), and α -GAL represents one of a small number of recombinant human proteins approved for the treatment of any disease. A second treatment for Fabry disease (specific for the cardiac variant of the disease) uses galactose infusion, which presumably helps stabilize the mutant α -GAL protein (Frustaci, A., et al., *N. Engl. J. Med.*, 2001, 345:25-32). In addition to enzyme replacement therapy and galactose infusion, gene replacement therapy using the α -GAL gene shows potential as a treatment for Fabry disease (Park, J., et al., *Proc Natl Acad Sci U S A*, 2003, 100:3450-4).

10

There are currently two recombinant glycoprotein products, REPLAGALTM (Transkaryotic Therapies, Inc., Cambridge, MA) and FABRAZYMETM (Genzyme, Inc., Cambridge, MA), available for enzyme replacement therapy used in the treatment of Fabry disease (Schiffmann, R., et al., *JAMA*, 2001, 285:2743-9; Eng, C. M., et al., *N. Engl. J. Med.*, 2001, 345:9-16). These two glycoproteins have identical amino acid sequences but are produced in different cell lines, resulting in different glycosylation at the N-linked carbohydrate attachment sites. REPLAGALTM is produced in a genetically engineered human cell line, while FABRAZYMETM is produced in a Chinese hamster ovary (CHO) cell line. REPLAGALTM contains a greater amount of complex carbohydrate while Fabrazyme contains a higher fraction of sialylated and phosphorylated carbohydrate (Lee, K., et al., *Glycobiology*, 2003, 13:305-13). Because the polypeptide sequence of the two glycoproteins is identical, these differences in carbohydrate composition are solely responsible for the differences in tissue distribution and dose response of the two enzyme replacement therapies.

α-GAL has also attracted attention for its ability to convert human blood group antigens. Recombinant α-GAL has been used to convert blood of type B into blood of type O, the universal donor type (Zhu, A., et al., Arch. Biochem. Biophys., 1996, 327:324-9), a process currently in clinical trials.

Because of its utility in the treatment of Fabry disease and as a reagent for converting human blood types, much effort has been put into the expression and purification of large amounts of human α-GAL. The endogenous enzyme has been purified from human placenta (Mayes, J. S. & Beutler, E., *Biochim Biophys Acta*, 1977, 484:408-16), liver cells (Dean, K. J. & Sweeley, C. C., *J Biol Chem*, 1979, 254:9994-10000), spleen cells and plasma (Bishop, D. F. & Desnick, R. J., *J Biol Chem*, 1981, 256:1307-16), and fibroblasts (Lemansky, P., et al., *J Biol Chem*, 1987, 262:2062-5); recombinant enzyme has been produced in *E. coli* bacterial

cells (Hantzopoulos, P. A. & Calhoun, D. H., *Gene*, 1987, 57:159-69), COS monkey cells (Tsuji, S., et al., *Eur J Biochem*, 1987, 165:275-80), CHO cells (Ioannou, Y. A., et al., *J Cell Biol*, 1992, 119:1137-50), baculovirus-infected Sf9 insect cells (Coppola, G., et al., *Gene*, 1994, 144:197-203; Chen, Y., et al., *Protein Expr Purif*, 2000, 20:228-36), *Pichia pastoris* yeast cells (Chen, Y., et al., *Protein Expr Purif*, 2000, 20:472-84), transduced human bone marrow cells (Takenaka, T., et al., *Exp Hematol* 1999, 27:1149-59), and continuously cultured genetically engineered human fibroblasts (Schiffmann, R., et al., *JAMA*, 2001, 285:2743-9). Despite the ability to successfully express and purify human α-GAL since 1977, the three-dimensional structure has not been solved, although a crystallization report appeared in 1994 (Murali, R., et al., *J. Mol. Biol.* 239:578-80). Structural analysis has been hindered by the heterogeneous carbohydrates on the glycoprotein, which comprise 5-15% of the mass of the secreted material and contain over 70 different species built upon 23 different core structures (Matsuura, F., et al., *Glycobiology* 1998, 8:329-39).

Thus, there is a great need to solve the crystal structure of α -GAL and, in particular, to delineate the active site of the enzyme. With this information, computer models of this active/binding site can be created and potential agonists and antagonists of α -GAL can be rationally designed.

15

20

25

Summary of the Invention

This invention provides the crystal structure of human α -GAL. The crystal structure has been solved by X-ray crystallography to a resolution of 3.25 Å. Based upon the crystal structure we have characterized human α -GAL in detail and identified the key amino acid residues that make up the active/binding site of the enzyme. These coordinates are useful in methods for designing agonists and antagonists of the enzyme, which in turn may be useful in treating Fabry and other diseases.

The invention also provides the X-ray structure coordinates of a complex comprising α -GAL and its catalytic product, α -galactose.

In another aspect the invention provides a computer programmed with the coordinates of the human α -GAL active/binding site, and with a program capable of converting those coordinates into a three-dimensional representation of the active site on a display connected to the computer.

In a further aspect, the invention provides a computer which, when programmed with at least a portion of the structural coordinates of human α -GAL and an X-ray diffraction data

set of a different molecule or molecular complex, performs a Fourier transform of these structural coordinates of the human α -GAL coordinates and then processes the X-ray diffraction data into structure coordinates of the different molecule or molecular complex via the process of molecular replacement.

These and other objects of the invention will be described in further detail in connection with the detailed description of the invention.

Brief Description of the Sequences

SEQ ID NO:1 is the nucleotide sequence of the human α -GAL cDNA.

5

10

15

20

25

30

SEQ ID NO:2 is the predicted amino acid sequence of the translation product of human α -GAL cDNA (SEQ ID NO:1).

Brief Description of the Drawings

- FIG. 1 (pp. 1-82) lists the atomic structure coordinates for human α -GAL as derived by X-ray diffraction from a crystal of human α -GAL dimer. The following abbreviations are used in FIG. 1: "Atom type" refers to the element whose coordinates are measured. The first letter in the column defines the element.
 - "X, Y, Z" crystallographically define the atomic position of the element measured.
- "OCC" is an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i.e., the same position, in all molecules of the crystal.
 - "B" is a thermal factor that measures movement of the atom around its atomic center.
- FIG. 2 shows a diagram of a computer used to generate a three-dimensional graphical representation of a molecule or molecular complex according to this invention.
 - FIG. 3 shows a cross section of a magnetic storage medium.
 - FIG. 4 shows a cross section of an optically-readable data storage medium.
- FIG. 5 is a schematic showing the reaction catalyzed by α -GAL; FIG. 5(a) the general reaction of α -GAL; FIG. 5 (b) α -GAL and Fabry disease.
- FIG. 6 depicts a stereo ribbon diagram of the overall fold of: (a) the α -GAL monomer; (b) and (c) the α -GAL dimer (two views); (d) the surface of α -GAL.
 - FIG. 7 is a phylogeny tree depicting the evolutionary relationships in the α -GAL/ α -NAGAL family.

FIG. 8 depicts electron density maps showing the active site of human α -GAL from (a) native and (b) galactose-soaked crystals; FIG. 8 (c) shows the superimposed active sites of human α -GAL (green), and chicken α -NAGAL (yellow).

FIG. 9 depicts the N-linked carbohydrate attached to N192 of human α -GAL is shown with helix α 4. Electron density from a σ_A -weighted simulated annealing composite omit map (grey) is contoured at 1.1 σ . Five sugar residues have been built into the electron density at this site.

FIG. 10 is a schematic representation of the human $\alpha\text{-GAL}$ active site with a galactose molecule.

Detailed Description of the Invention

10

20

As mentioned above, we have solved the three-dimensional X-ray crystal structure of human α -galactosidase. The atomic coordinate data is presented in FIG. 1.

In order to use the structure coordinates generated for the human α -galactosidase, its active site or portions or homologues thereof, it is often times necessary to convert them into a three-dimensional shape. This is achieved through the use of commercially available software that is capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of structure coordinates.

An "active site", also referred to as "binding site" elsewhere herein, is of significant utility in fields such as drug discovery. The association of natural ligands or substrates with the active site(s) (or "binding pocket") of their corresponding receptors or enzymes is the basis of many biological mechanisms of action. Similarly, many drugs exert their biological effects through association with the binding pockets of receptors and enzymes. Such associations may occur with all or any parts of the binding pocket. An understanding of such associations will help lead to the design of drugs having more favorable associations with their target receptor or enzyme, and thus, improved biological effects. Therefore, this information is valuable in designing potential agonists and antagonists of the binding sites of biologically important targets.

The term "active site" (or "binding pocket"), as used herein, refers to a specific region of an enzyme, that, as a result of its shape, favorably associates with its substrate and catalysis occurs.

We have identified at least one active site per monomer in human α -GAL, which is a good target for designing agonists and/or antagonists and/or inhibitors.

The terms " α -GAL-like binding pocket", as used herein, refers to a portion of a molecule or molecular complex whose shape is sufficiently similar to the human α -GAL binding pocket, so as to bind common ligands. These commonalties of shape are defined by a root mean square deviation from the structure coordinates of the backbone atoms of the amino acids that make up these binding pockets in the human α -GAL structure (as set forth in FIG. 1) of not more than 1.5 Å. The method of performing this calculation is described below.

The x-ray structure reveals human α-GAL as a homodimeric glycoprotein with each monomer composed of two domains, a $(\beta/\alpha)_8$ domain containing the active site and a Cterminal domain containing eight antiparallel β strands on two sheets in a β sandwich (FIG. 6a). After removal of the 31 residue signal sequence, the first domain extends from residues 32 to 330 and contains the active site formed by the C-terminal ends of the β strands at the center of barrel, a typical location for the active site in $(\beta/\alpha)_8$ domains. The second domain, comprised of residues 331 to 429, packs against the first with an extensive interface, burying 2500 Å² of surface area within one monomer. The dimer has overall protein dimensions of approximately 75 x 75 x 50Å (FIG. 6b). The molecule is concave in the third dimension and varies in thickness from approximately 20 to 50Å (FIG. 6c). Electron density is visible for 390 and 391 amino acid residues (out of 398 total) in the two copies of the monomer in the crystallographic asymmetric unit; the missing residues occur at the C-terminus. The two monomers pack with an interface that extends the 75Å width of the dimer and buries 2200 Å² of surface area. In the dimer interface, 30 residues from each monomer contribute to the interface, from loops $\beta 1-\alpha 1$, $\beta 6-\alpha 6$, $\beta 7-\alpha 7$, $\beta 8-\alpha 8$, $\beta 11-\beta 12$, and $\beta 15-\beta 16$. The dimer is markedly negatively charged, as seen in a surface electrostatic potential (FIG. 6d). With 47 carboxylate groups and only 36 basic residues in the 398 residues in the molecule, the overall charge per monomer is expected to be -11 at neutral pH. The carboxylates are most concentrated around the active site, but in the low pH of the lysosome, many of these groups become protonated, reducing the charge on the molecule. In addition to the negative charges on the protein, the N-linked carbohydrate is highly phosphorylated and sialylated (Lee, K., et al., Glycobiology, 2003, 13:305-13) (see below), further increasing its negative electrostatic potential. The N-linked carbohydrates fall distal to the active sites (FIG. 6d). Each monomer contains the three N-linked carbohydrate sites, five disulfide bonds (C52-C94, C56-C63, C142-C172, C202-C223, and C378-C382), two unpaired cysteines (C90 and C174), and three cis prolines (P210, P380, and P389).

20

As mentioned above, the C-terminal seven and eight residues of each chain have no electron density associated with them and are presumably disordered. This disorder is consistent with the observation of slight heterogeneity in the C-terminus of recombinant human α -GAL, where the truncation of one or two residues from the C-terminus can occur but has no effect upon the activity of the enzyme (Lee, K., et al., *Glycobiology*, 2003, 13:305-13). The structure offers no support for the observation that the removal of 2 to 10 residues from the C-terminus increases the activity of α -GAL (Miyamura, N., et al., *J Clin Invest*, 1996, 98:1809-17), because the final residue seen in the structure falls at least 45Å from each active site and on the opposite face of the molecule.

10

25

In both the native and galactose-soaked crystal structures, electron density appears in the two crystallographically-independent active sites (FIGS. 8a and b). In the galactose-soaked crystal, this density represents α-galactose, the normal catalytic product of the enzyme (K_i ~1mM). In the native structure, this density most likely derives from the cryoprotectant ethylene glycol, a weak inhibitor of glycoside hydrolases (Tsitsanou, K. E., et al., *Protein Sci*, 1999, 8:741-9), analogous to the insertion of glycerol into carbohydrate binding sites on proteins (Garman, S. C., et al., *Structure*, 2002, 10:425-434; Tsitsanou, K. E., et al., *Protein Sci*, 1999, 8:741-9; Schmidt, A., et al., *Protein Sci*, 1998, 7:2081-8). The two active sites of the dimer are separated by approximately 50 Å. As the enzyme shows little change between the liganded and unliganded structures, there is no evidence for cooperativity between the two sites, although the biochemical evidence is mixed (Dean, K. J. & Sweeley, C. C., *J Biol Chem*, 1979, 254:9994-10000; Bishop, D. F. & Desnick, R. J., *J Biol Chem*, 1981, 256:1307-16).

We have determined that human α -GAL binds α -galactose by making specific contacts to each functional group on the monosaccharide. Residues from seven loops in domain 1 form the *active site*: β 1- α 1, β 2- α 2, β 3- α 3, β 4- α 4, β 5- α 5, β 6- α 6, and β 7- α 7. The active site is formed by the side chains of residues W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267. Thus, a binding pocket defined by the structural coordinates of these amino acids, as set forth in FIG. 1; or a binding pocket whose root mean square deviation from the structure coordinates of the backbone atoms of these amino acids is not more than 1.5 Å is considered a human α -GAL-like binding pocket of this invention. In important embodiments, C172 makes a disulfide bond to C142.

In the α -GAL/ α -NAGAL family, specificity for the 2 position on the galactose ligand occurs via the β 5- α 5 loop. This was called the "N-acetyl recognition loop" in α -NAGAL

(Garman, S. C., et al., *Structure*, 2002, 10:425-434); in the overall α -GAL/ α -NAGAL family "2 position recognition loop" or "2 loop" is appropriate. This loop falls near the boundary of exons 4 and 5 of animal α -GAL/ α -NAGAL, which have a small insertion in this region, resulting in a short helical stretch at the top of the β 5 strand; this insertion is absent in other species. Plant and fungal α -GALs use a Cys and a Trp on this loop to coordinate the 2-hydroxyl on galactose; animal α -GAL uses a Glu and a Leu to recognize the 2-hydroxyl (FIG. 7, green) while animal α -NAGAL uses a Ser and an Ala to recognize an N-acetyl at the 2 position (FIG. 7, yellow). In the animal enzymes, the larger Glu and Leu side chains sterically block the larger N-acetyl substituent, while the smaller Ser and Ala side chains nicely accommodate an N-acetyl group and tolerate a hydroxyl group.

With three different conformations in the 2 loop now identified, the substrate specificity of the other members of the family can be categorized by homology. For example, genome sequencing of *Drosophila melanogaster* and *Anopheles gambiae* have each identified pairs of genes in the α -GAL family. By examination of the sequences in the 2 loop, two are clearly α -NAGALs while the other two appear to be α -GALs (FIG. 7, yellow and purple). Surprisingly, *Aspergillus niger* contains an enzyme identified as α -GAL that, although only 30% identical to the animal protein sequences, contains a 2 loop virtually identical to animal α -NAGALs (FIG. 7, yellow). We predict this enzyme is primarily an α -NAGAL with partial α -GAL activity, much like human α -NAGAL, which was originally thought to be an α -GAL based upon similar activity (Dean, K. J., et al., *Biochem. Biophys. Res. Commun.*, 1977, 77:1411-7; Schram, A. W., et al., *Biochim. Biophys. Acta*, 1977, 482:138-44).

20

Although human α -GAL makes contacts to each functional group on the α -galactose ligand, the enzyme shows little specificity for the distal portion of the substrate beyond the glycosidic linkage, and the active site cleft is found in a broad opening on the concave surface of the enzyme (FIG. 6c). The lack of substrate specificity of human α -GAL beyond the terminal α -galactose differs slightly from the specificity of other α -GALs, which act only upon substrates containing terminal α 1-6 galactose groups (Kim,W.D., et al., *Phytochemistry*, 2002, 61:621-30). This increased specificity of plant α -GALs may derive from their monomeric structure, as residues buried in the dimer interface of animal α -GALs (e.g., those on the β 1- α 1 loop - Fujimoto, Z., et al., *J Biol Chem*, 2003, 278:20313-8) are available for ligand recognition in monomeric α -GALs.

Both α -GALs and α -NAGALs are α retaining exoglycosidases, where both the substrate and product of the catalytic reactions are α anomers at the 1 position on the galactose ring. This retention of anomeric configuration is accomplished by a double displacement catalytic mechanism where the anomeric carbon undergoes two successive nucleophilic attacks (Vasella, A., et al., Curr Opin Chem Biol, 2002, 6:619-29). The two sequential inversions of the anomeric carbon lead to retention of the configuration at the end of the catalytic cycle. In two α-GALs from different species, peptic digestion of covalently trapped intermediates has identified the specific aspartic acid acting as the catalytic nucleophile (Hart, D. O., et al., Biochemistry, 2000, 39:9826-36; Ly, H. D., et al., Carbohydr. Res., 2000, 329:539-47). These data, combined with the high resolution structure of chicken α -NAGAL, predict the catalytic mechanism of human α -GAL. In human α -GAL, the first nucleophilic attack upon the substrate comes from D170, cleaving the glycosidic linkage and leading to a covalent enzyme-intermediate complex. In the second step of the reaction, a water molecule (deprotonated by D231) attacks C1 of the covalent intermediate, liberating the second half of the catalytic product and regenerating the enzyme in its initial state. Human α-GAL operates most efficiently at low pH, consistent with its highly acidic composition and its lysosomal location.

Retaining glycosidases typically have distances of 5-6Å between catalytic carboxylates, while inverting glycosidases typically have distances of 9-11Å between these residues (McCarter, J. D. & Withers, S. G., Curr. Opin. Struct. Biol. 1994, 4:885-92). From these distances, it has been possible to reliably predict the mechanism and function of a glycosidase given its structure. However, this rule must be reconsidered in light of the new structures in the α -GAL/ α -NAGAL family: for the known structures in the family, the closest approach of the two catalytic carboxylates is 6.5-7Å, among the largest distances seen for retaining glycosidases.

25

It will be readily apparent to those of skill in the art that the numbering of amino acids in other isoforms of human α -GAL may be different than that set forth for herein. Corresponding amino acids in other isoforms of human α -GAL are easily identified by visual inspection of the amino acid sequences or by using commercially available homology software programs. Each of those amino acids of human α -GAL is defined by a set of structure coordinates set forth in FIG. 1. The term "structure coordinates" refers to Cartesian coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a protein

or protein-ligand complex in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are then used to establish the positions of the individual atoms of the enzyme or enzyme complex.

Those of skill in the art understand that a set of structure coordinates for an enzyme or an enzyme-complex or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates will have little effect on overall shape. In terms of binding pockets, these variations would not be expected to significantly alter the nature of ligands that could associate with those pockets.

The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and a binding pocket or binding site on a protein. The association may be non-covalent--wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions--or it may be covalent.

10

15

20

25

30

The variations in coordinates discussed above may be generated because of mathematical manipulations of the human α -GAL structure coordinates. For example, the structure coordinates set forth in FIG. 1 could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above.

Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal could also account for variations in structure coordinates. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be the same. Thus, for example, a ligand (e.g., substrate) that bound to the α -GAL active site would also be expected to bind to another binding pocket whose structure coordinates defined a shape that fell within the acceptable error.

Various computational analyses are therefore necessary to determine whether a molecule or the binding pocket portion thereof is sufficiently similar to the α-GAL active/binding site described above. Such analyses may be carried out in well known software applications, such as the Molecular Similarity application of QuantaTM (Molecular Simulations Inc., San Diego, CA.) version 4.1, and as described in the accompanying User's Guide.

The Molecular Similarity application permits comparisons between different structures, different conformations of the same structure, and different parts of the same structure. The procedure used in Molecular Similarity to compare structures is divided into four steps: 1) load the structures to be compared; 2) define the atom equivalences in these structures; 3) perform a fitting operation; and 4) analyze the results.

Each structure is identified by a name. One structure is identified as the target (i.e., the fixed structure); all remaining structures are working structures (i.e., moving structures). Since atom equivalency within QuantaTM is defined by user input, for the purpose of this invention we will define equivalent atoms as protein backbone atoms (N, Cα, C and O) for all conserved residues between the two structures being compared. We also consider only rigid fitting operations.

When a rigid fitting method is used, the working structure is translated and rotated to obtain an optimum fit with the target structure. The fitting operation uses an algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in angstroms (Å), is reported by QuantaTM.

15

20

25

30

For the purpose of this invention, any molecule or molecular complex or binding pocket thereof that has a root mean square deviation of conserved residue backbone atoms (N, Ca, C and O) of less than 1.5 Å when superimposed on the relevant backbone atoms described by structure coordinates listed in FIG. 1 are considered identical. More preferably, the root mean square deviation is less than 1.0 Å.

The term "root mean square deviation" means the square root of the arithmetic mean of the squares of the deviations from the mean. It is a way to express the deviation or variation from a trend or object. For purposes of this invention, the "root mean square deviation" defines the variation in the backbone of a protein from the backbone of human α -GAL or a binding pocket portion thereof, as defined by the structure coordinates of human α -GAL described herein.

Therefore, according to one aspect of the invention a computer is provided for producing:

(a) a three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises a binding pocket defined by structure coordinates of human α-galactosidase amino acids W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1; or

b) a three-dimensional representation of a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, wherein said computer comprises:

5

10

15

25

30

- a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the structure coordinates of human α-galactosidase amino acids W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1;
- (ii) a working memory for storing instructions for processing said machinereadable data;
- (iii) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data into said three-dimensional representation; and
- (iv) a display coupled to said central-processing unit for displaying said threedimensional representation.

In an important embodiment, C172 makes a disulfide bond to C142.

According to another aspect of the invention, a computer for producing a three-dimensional representation of a molecule or molecular complex defined by structure coordinates of all of the human α -GAL amino acids set forth in FIG. 1, or a three-dimensional representation of a homologue of said molecule or molecular complex, is provided. The homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å. In this aspect of the invention, a machine readable data contains the coordinates of all of human α -GAL.

According to a further aspect, the invention provides a computer for determining at least a portion of the structure coordinates corresponding to X-ray diffraction data obtained from a molecule or molecular complex, wherein said computer comprises:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structural coordinates of human α -GAL according to FIG. 1;

- (b) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises X-ray diffraction data from said molecule or molecular complex;
- (c) a working memory for storing instructions for processing said machine-readable data of (a) and (b);
 - (d) a central-processing unit coupled to said working memory and to said machinereadable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structure coordinates; and
 - (e) a display coupled to said central-processing unit for displaying said structure coordinates of said molecule or molecular complex.

10

20

30

FIG. 2 demonstrates one version of the foregoing aspects. System 10 includes a computer 11 comprising a central processing unit ("CPU") 20, a working memory 22 which may be, e.g., RAM (random-access memory) or "core" memory, mass storage memory 24 (such as one or more disk drives or CD-ROM drives), one or more cathode-ray tube ("CRT") display terminals 26, one or more keyboards 28, one or more input lines 30, and one or more output lines 40, all of which are interconnected by a conventional bi-directional system bus 50.

Input hardware 36, coupled to computer 11 by input lines 30, may be implemented in a variety of ways. Machine-readable data of this invention may be inputted via the use of a modern or moderns 32 connected by a telephone line or dedicated data line 34. Alternatively or additionally, the input hardware 36 may comprise CD-ROM drives or disk drives 24. In conjunction with display terminal 26, keyboard 28 may also be used as an input device.

Output hardware 46, coupled to computer 11 by output lines 40, may similarly be implemented by conventional devices. By way of example, output hardware 46 may include CRT display terminal 26 for displaying a graphical representation of a binding pocket of this invention using a program such as QuantaTM as described herein. Output hardware might also include a printer 42, so that hard copy output may be produced, or a disk drive 24, to store system output for later use.

In operation, CPU 20 coordinates the use of the various input and output devices 36, 46, coordinates data accesses from mass storage 24 and accesses to and from working memory 22, and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are

discussed in reference to the computational methods of drug discovery as described herein. Specific references to components of the hardware system 10 are included as appropriate throughout the following description of the data storage medium.

FIG. 3 shows a cross section of a magnetic data storage medium 100 which can be encoded with a machine-readable data that can be carried out by a system such as system 10 of FIG. 2. Medium 100 can be a conventional floppy diskette or hard disk, having a suitable substrate 101, which may be conventional, and a suitable coating 102, which may be conventional, on one or both sides, containing magnetic domains (not visible) whose polarity or orientation can be altered magnetically. Medium 100 may also have an opening (not shown) for receiving the spindle of a disk drive or other data storage device 24.

The magnetic domains of coating 102 of medium 100 are polarized or oriented so as to encode in manner which may be conventional, machine readable data such as that described herein, for execution by a system such as system 10 of FIG. 2.

FIG. 4 shows a cross section of an optically-readable data storage medium 110 which also can be encoded with such a machine-readable data, or set of instructions; which can be carried out by a system such as system 10 of FIG. 2. Medium 110 can be a conventional compact disk read only memory (CD-ROM) or a rewritable medium such as a magneto-optical disk which is optically readable and magneto-optically writable. Medium 100 preferably has a suitable substrate 111, which may be conventional, and a suitable coating 112, which may be conventional, usually of one side of substrate 111.

In the case of CD-ROM, as is well known, coating 112 is reflective and is impressed with a plurality of pits 113 to encode the machine-readable data. The arrangement of pits is read by reflecting laser light off the surface of coating 112. A protective coating 114, which preferably is substantially transparent, is provided on top of coating 112.

20

25

In the case of a magneto-optical disk, as is well known, coating 112 has no pits 113, but has a plurality of magnetic domains whose polarity or orientation can be changed magnetically when heated above a certain temperature, as by a laser (not shown). The orientation of the domains can be read by measuring the polarization of laser light reflected from coating 112. The arrangement of the domains encodes the data as described above.

Thus, in accordance with the present invention, X-ray coordinate data capable of being processed into a three dimensional graphical display of a molecule or molecular complex which comprises an α -GAL-like binding pocket is stored in a machine-readable storage medium.

The human α -GAL X-ray coordinate data, when used in conjunction with a computer programmed with software to translate those coordinates into the 3-dimensional structure of a molecule or molecular complex comprising an α -GAL-like binding pocket may be used for a variety of purposes, such as drug discovery.

For example, the structure encoded by the data may be computationally evaluated for its ability to associate with chemical entities. Chemical entities that associate with human α -GAL may inhibit that enzyme, and are potential drug candidates. Alternatively, the structure encoded by the data may be displayed in a graphical three-dimensional representation on a computer screen. This allows visual inspection of the structure, as well as visual inspection of the structure's association with chemical entities.

5

10

15

20

25

30

Thus, according to another aspect the invention relates to a method for evaluating the potential of a chemical entity to associate with:

- a) a molecule or molecular complex comprising a binding pocket defined by structure coordinates of human α-galactosidase amino acids W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1, or
- b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å. The method comprises the steps of:
- i) employing computational means to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex; and
- ii) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket.

The term "chemical entity," as used herein, refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes.

Alternatively, the structural coordinates of the human α -GAL binding pocket can be utilized in a method for identifying a potential agonist or antagonist of a molecule comprising a human α -GAL-like binding pocket. The method comprises the steps of:

a) using the atomic coordinates of human α -galactosidase amino acids W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1 \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, to generate a three-dimensional structure of molecule comprising α -GAL-like binding pocket;

- b) employing said three-dimensional structure to design or select said potential agonist or antagonist;
 - c) synthesizing said agonist or antagonist; and

5

10

. 15

20

25

d) contacting said agonist or antagonist with said molecule to determine the ability of said potential agonist or antagonist to interact with said molecule.

In important embodiments, the atomic coordinates of all the amino acids of NS3 human α -GAL according to FIG. 1 \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, are used to generate a three-dimensional structure of molecule comprising an α -GAL-like binding pocket.

For the first time, the present invention permits the use of molecular design techniques to identify, select and design chemical entities, including agonists and antagonists, capable of binding to human α -GAL-like binding pockets. Because of the present invention, the necessary information for designing new chemical entities and compounds that may interact with human α -GAL-like binding pockets, in whole or in part, is provided.

Throughout this section, discussions about the ability of an entity to bind to, associate with or inhibit a human α -GAL-like binding pocket refers to features of the entity alone. Assays to determine if a compound binds to human α -GAL are well known in the art and are exemplified below.

The design of compounds that bind to or inhibit human α -GAL-like binding pockets according to this invention generally involves consideration of two factors. First, the entity must be capable of physically and structurally associating with parts or all of the human α -GAL -like binding pockets. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions and electrostatic interactions.

Second, the entity must be able to assume a conformation that allows it to associate with the human α -GAL-like binding pocket directly. Although certain portions of the entity will not directly participate in these associations, those portions of the entity may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, or the spacing between functional groups of an entity comprising several chemical

entities that directly interact with the human α -GAL-like binding pocket or homologues thereof.

The potential inhibitory or binding effect of a chemical entity on a human α -GAL-like binding pocket may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given entity suggests insufficient interaction and association between it and the human α -GAL-like binding pocket, testing of the entity is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to a human α -GAL-like binding pocket. This may be achieved by testing the ability of the molecule to inhibit human α -GAL using assays described in the art. In this manner, synthesis of inoperative compounds may be avoided.

A potential inhibitor of a human α -GAL-like binding pocket may be computationally evaluated by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the human α -GAL-like binding pockets.

15

25

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with a human α -GAL-like binding pocket. This process may begin by visual inspection of, for example, a human α -GAL-like binding pocket on the computer screen based on the human α -GAL structure coordinates in FIG. 1 or other coordinates which define a similar shape generated from the machine-readable storage medium. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within that binding pocket as defined supra. Docking may be accomplished using software such as QuantaTM and SybylTM, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CharmmTM and AmberTM.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include: GRID (P. J. Goodford, *J. Med. Chem.*, 1985, 28:849-857), available from Oxford University, Oxford, UK; MCSS (A. Miranker et al., *Proteins: Structure, Function and Genetics*, 1991, 11:29-34), available from Molecular Simulations, San Diego, CA; AUTODOCK (D. S. Goodsell et al., *Proteins: Structure. Function, and Genetics*, 1990, 8:195-20), available from Scripps Research Institute, La Jolla, CA; DOCK (I. D. Kuntz et al., *J. Mol. Biol.*, 1982, 161:269-288), available from University of California, San Francisco, CA.

Other suitable software that can be used to view, analyze, design, and/or model a protein, and/or protein fragments, include but are not limited to: Alchemy™, LabVision™, Sybyl™, Molcadd™, Leapfrog™, Matchmaker™, Genefold™ and Sitel™ (available from Tripos Inc., St. Louis, MO); QuantaTM, Cerius2TM, X-PlorTM, CNSTM, CatalystTM, Modeller™, ChemX™, Ludi™, Insight™, Discover™, Cameleon™ and Iditis™ (available from Accelrys Inc., Princeton N.J.); Rasmol™ (available from Glaxo Research and Development, Greenford, Middlesex, U.K.); MOETM (available from Chemical Computing Group, Montreal, Quebec, Canada); MaestroTM (available from Shrodinger Inc.,); Midas/MidasPlus™ (available from UCSF, San Francisco, CA); VRML (webviewer-freeware on the internet); Chime (MDL--freeware on the internet); MOIL (available from University of Illinois, Urbana-Champaign, IL); MacroModel™ and GRASP™ (available from Columbia University, New York, NY); Ribbon™ (available from University of Alabama, Tuscaloosa, AL); NAOMITM (available from Oxford University, Oxford, UK); Explorer EyechemTM (available from Silicon Graphics Inc., Mountain View, CA); Univision[™] (available from Cray Research Inc., Seattle, WA); Molscript[™] and O (available from Uppsala University, Uppsala, Sweden); Chem 3D™ and Protein Expert™ (available from Cambridge Scientific, MA); ChainTM (available from Baylor College of Medicine, Houston, TX); Spartan™, MacSpartan™ and Titan™ (available from Wavefunction Inc., Irvine, CA); VMD™ (available from U. Illinois/Beckman Institute); Sculpt™ (available from Interactive Simulations, Inc., Portland, OR); ProcheckTM (available from Brookhaven National Laboratory, Upton, NY); DGEOM (available from QCPE--Quantum Chemistry Program Exchange, Indiana University Bloomington, IN); RE_VIEW (available from Brunel University, London, UK); Xmol (available from Minnesota Supercomputing Center, University of Minnesota, Minneapolis, MN); Hyperchem[™] (available from Hypercube, Inc., Gainesville, FL); MD Display (available from University of Washington, Seattle, WA.); PKB (available from National Center for Biotechnology Information, NIH, Bethesda, MD); Molecular Discovery Programmes (available from Molecular Discovery Limited, Mayfair, London); Growmol™ (available from Thistlesoft, Morris Township, N.J.); MICE (available from The San Diego Supercomputer Center. La Jolla, CA); Yummie and MCPro (available from Yale University, New Haven, CT); CaveatTM (P. A. Bartlett et al, In "Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 1989, 78:182-196; G. Lauri and P. A. Bartlett, J. Comput. Aided Mol. Des., 1994, 8:51-66), available from the University of California, Berkeley, CA; 3D Database systems such as

20

ISIS™ (MDL Information Systems, San Leandro, CA). This area is reviewed in Y. C. Martin, "3D Database Searching in Drug Design", J. Med. Chem., 1992, 35:2145-2154; Hook™ (M. B. Eisen et al, Proteins: Struct., Funct., Genet., 1994, 19:199-221), available from Molecular Simulations, San Diego, CA; and upgraded versions thereof.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of human α -GAL. This would be followed by manual model building using software such as QuantaTM or SybylTM.

5

15

20

Instead of proceeding to build an inhibitor of human α -GAL-like binding pocket in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other human α -GAL binding compounds may be designed as a whole or "de novo" using either an empty binding site or optionally including some portion(s) of a known inhibitor(s).

Other molecular modeling techniques may also be employed in accordance with this invention [see, e.g., N. C. Cohen et al., *J. Med. Chem.*, 1990, 33:883-894; see also, M. A. Navia and M. A. Murcko, *Curr. Opin. in Struct. Biology*, 1992, 2:202-210; L. M. Balbes et al., "A Perspective of Modern Methods in Computer-Aided Drug Design", in *Reviews in Computational Chemistry*, Vol. 5, K. B. Lipkowitz and D. B. Boyd, Eds., VCH, New York, pp. 337-380 (1994); see also, W. C. Guida, *Curr. Opin. Struct. Biology*, 1994, 4:777-781].

Once a compound has been designed or selected by the above methods, the efficiency with which that entity may bind to an human α -GAL binding pocket may be tested and optimized by computational evaluation. For example, an effective human α -GAL binding pocket inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient human α -GAL binding pocket inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, more preferably, not greater than 7 kcal/mole. Human α -GAL binding pocket inhibitors may interact with the binding pocket in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the inhibitor binds to the protein.

An entity designed or selected as binding to a human α -GAL binding pocket may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme and with the surrounding water molecules. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interactions. Examples of software designed for such uses include: Gaussian 94, revision C (M. J. Frisch, Gaussian, Inc., Pittsburgh, PA, @1995); AMBER, version 4.1 (P. A. Kollman, University of California at San Francisco, @1995); QUANTA/CHARMM (Molecular Simulations, Inc., San Diego, CA, @1995); Insight II/Discover (Molecular Simulations, Inc., San Diego, CA @1995); DelPhi (Molecular Simulations, Inc., San Diego, CA @1995); and AMSOL (Quantum Chemistry Program Exchange, Indiana University). These programs may be implemented, for instance, using a Silicon Graphics workstation such as an Indigo² with "IMPACT" graphics. Other hardware systems and software packages will be known to those skilled in the art.

Another approach enabled by this invention, is the computational screening of small molecule databases for chemical entities or compounds that can bind in whole, or in part, to a human α -GAL binding pocket. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy (E. C. Meng et al., *J. Comp. Chem.*, 1992, 13:505-524).

According to another embodiment, the invention provides compounds which associate with a human α -GAL-like binding pocket produced or identified by the method set forth above.

20

30

The structure coordinates set forth in FIG. 1 can also be used to aid in obtaining structural information about another crystallized molecule or molecular complex. This may be achieved by any of a number of well-known techniques, including molecular replacement.

Therefore, in another aspect this invention provides a method of utilizing molecular replacement to obtain structural information about a molecule or molecular complex whose structure is unknown comprising the steps of:

- a) crystallizing said molecule or molecular complex of unknown structure;
- b) generating X-ray diffraction data from said crystallized molecule or molecular complex; and

c) applying at least a portion of the structure coordinates set forth in FIG. 1 to the X-ray diffraction data to generate a three-dimensional electron density map of the molecule or molecular complex whose structure is unknown.

By using molecular replacement, all or part of the structure coordinates of the human α -GAL as provided by this invention (and set forth in FIG. 1) can be used to determine the structure of a crystallized molecule or molecular complex whose structure is unknown more quickly and efficiently than attempting to determine such information *ab initio*.

Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that can not be determined directly, obtaining accurate values for the phases, by methods other than molecular replacement, is a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure provide a satisfactory estimate of the phases for the unknown structure.

Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of the human α-GAL according to FIG. 1 within the unit cell of the crystal of the unknown molecule or molecular complex so as best to account for the observed X-ray diffraction data of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction data amplitudes to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule or molecular complex [E. Lattman, *Meth. Enzymol.*, 1985, 115:55-77; M. G. Rossmann, ed., "The Molecular Replacement Method", *Int. Sci. Rev. Ser.*, No. 13, Gordon & Breach, New York (1972)].

The structure of any portion of any crystallized molecule or molecular complex that is sufficiently homologous to any portion of human α -GAL can be resolved by this method.

In a preferred embodiment, the method of molecular replacement is utilized to obtain structural information about another galactosidase. The structure coordinates of human α -GAL as provided by this invention are particularly useful in solving the structure of other isoforms of α -GAL or other α -GAL-containing complexes.

30

Furthermore, the structure coordinates of human α -GAL as provided by this invention are useful in solving the structure of α -GAL proteins that have amino acid substitutions, additions and/or deletions (referred to collectively as "human α -GAL mutants", as compared to naturally occurring human α -GAL isoforms. These human α -GAL mutants may optionally be crystallized in co-complex with a chemical entity, such as galactose. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type human α -GAL. Potential sites for modification within the various binding sites of the enzyme may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between human α -GAL and a chemical entity or compound.

The structure coordinates are also particularly useful to solve the structure of crystals of human α -GAL or human α -GAL homologues co-complexed with a variety of chemical entities. This approach enables the determination of the optimal sites for interaction between chemical entities, including between candidate human α -GAL agonists and human α -GAL. For example, high resolution X-ray diffraction data collected from crystals exposed to different types of solvent allows the determination of where each type of solvent molecule resides. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their human α -GAL agonistic activity.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 1.5-3.5 Å resolution X-ray data to an R value of about 0.20 or less using computer software, such as X-PLOR [Yale University, ©1992, distributed by Molecular Simulations, Inc.; see, e.g., Blundell & Johnson, supra; Meth. Enzymol., vol. 114 & 115; H. W. Wyckoff et al., eds., Academic Press (1985)]. This α-GAL information thus be used to optimize known human may agonists/antagonists/inhibitors, and more importantly, to design new human α-GAL agonists/antagonists/inhibitors.

The invention will be more fully understood by reference to the following examples. These examples, however, are merely intended to illustrate the embodiments of the invention and are not to be construed to limit the scope of the invention.

25

Examples

Experimental Procedures Materials and Methods

Cloning and Expression of human α-Galactosidase:

Human α -Galactosidase (ReplagalTM lot G302-010, Transkaryotic Therapies, Inc.) was produced using gene activation technology as described in detail in U.S. Patents Nos. 5,733,761, 6,270,989, and 6,565,844, all of which are expressly incorporated herein by reference. Briefly, regulatory (e.g., a viral promoter) and structural DNA sequences were inserted upstream of the endogenous human α -Galactosidase genomic locus (GenBank Acc. No. HSU78027) in a human cell (e.g., HT-1080) using homologous recombination. As a result, α -Galactosidase expression was enhanced resulting in secretion of α -Galactosidase protein to the culture supernatant. The α -Galactosidase polypeptide was then highly purified using the methods described in detail in U.S. Patents Nos. 6,083,725, 6,395,884 and 6,458,574, all of which are expressly incorporated herein by reference.

Crystallization and x-ray data collection:

20

Human α-Galactosidase was concentrated to 40mg/ml in 20mM TrisHCl pH 7.5 prior to crystallization trials. Crystals were grown in either hanging or sitting drops via vapor diffusion against a reservoir solution of 30% polyethylene glycol (PEG) 4000 (Fluka), 100mM TrisHCl pH 8.0, and 200mM ammonium sulfate. Crystals were then harvested into 35% PEG 4000, 100mM TrisHCl pH 7.5, and 20% (v:v) ethylene glycol. Crystals were cooled in liquid nitrogen and then transferred into a gaseous nitrogen stream at 100K for xray data collection. Ligand-soaked crystals were transferred into 31% PEG 3350, 100mM sodium acetate pH 5.5, and 110mM D-(+)-galactose (Sigma) prior to nitrogen cooling and xray data collection. Despite efforts to increase their size, the crystals never grew larger than 30 x 30 x 100 μm. For each crystal, 180° of diffraction data were collected at beamline 22-ID at the Advanced Photon Source. Processing of x-ray images using the HKL2000 package (Otwinowski, Z. & Minor, W., Methods in Enzymology, 1997, 276:307-326) revealed unit cell constants of approximately 89Å x 89Å x 215Å in space P3₁21 or P3₂21. The diffraction from these crystals proved to be extremely anisotropic, with reflections visible to 2.8Å in the direction of the crystallographic c axis, but only to approximately 4Å in the perpendicular directions. This, plus the high redundancy and weak diffraction overall from the small crystals, resulted in very poor merging statistics. The native frames were initially processed using HKL2000 to 3.25Å. Reprocessing the frames in MOSFLM and SCALA (Collaborative Computational Project, *Acta Crystallogr.*, 1994, D50:760-763) with anisotropic diffraction limits produced maps of lower quality, so this route was abandoned, and the original data were used throughout the refinement. The high resolution limits were determined from the shell where <I/o

| dropped to 2. Intensities were adjusted with TRUNCATE (Collaborative Computational Project, *Acta Crystallogr.*, supra) prior to molecular replacement and refinement.

Phasing, model building, and refinement:

10

25

Molecular replacement calculations were performed in the program AmoRe (Collaborative Computational Project, Acta Crystallogr., 1994, D50:760-763) using a homology model of the human α-GAL protein built from the crystal structure of chicken α-NAGAL (Garman, S. C., et al., Structure, 2002, 10:425-434). The dimeric model was rotated and translated against the 8-4Å diffraction amplitudes. Molecular replacement in both enantiomorphic space group possibilities identified a dimer of α-GAL in the asymmetric unit of space group P3₂21 as the top solution, with a correlation coefficient of 28 and an R_{factor} of 58. Inspection of the packing showed no steric clashes in a unit cell with 50% solvent content. Rigid body refinement in the programs AMoRe and CNS (Brünger, A. T., et al., Acta Crystallogr. D Biol. Crystallogr. 1998, 54:905-21) was followed by model building in the program O (Jones, T. A., et al., Acta Crystallogr., 1991, A47:110-9). Residue numbering of the α -GAL protein begins at the secretory signal; the mature protein begins at amino acid 32. Refinement protocols in CNS included conjugate gradient minimization, simulated annealing, and temperature factor refinement. Models were built into σ_{A} weighted simulated annealing composite omit maps calculated in CNS. Strong two-fold non-crystallographic symmetry restraints (300 kcal/mol-Å²) were imposed on all atoms in the early stages of refinement, and later relaxed for the atoms that differ between the two halves of the dimer, including those in crystal contacts and N-linked carbohydrate atoms. Refinement steps were accepted only if they reduced the R_{free} (of a test set comprised of 820 reflections, 5% of the total, selected using resolution shells). The R_{work} and R_{free} for the native structure are 26.2% and 30.1%, respectively, using all reflections. Because of the limited resolution, side chain rotamers were typically chosen during manual rebuilding to be consistent with the 1.9Å chicken α-NAGAL structure.

Sequence alignments, calculations, and figures:

Beginning with the human α-GAL sequence, a BLAST search (Altschul, S. F., et al., Nucleic Acids Res 1997, 25:3389-402) of the NCBI non-redundant protein sequence database found the 50 closest sequences. After removal of 10 highly redundant sequences, the remaining 40 sequences were multiply aligned in CLUSTALW (Thompson, J. D., et al., Nucleic Acids Res, 1994, 22:4673-80), then converted into a phylogeny tree using the programs WEIGHBOR (Bruno, W. J., et al., Mol Biol Evol, 2000, 17:189-97) and PHYLIP (Felsenstein, J., Phylogeny Inference Package version 3.6, 1995, Department of Genetics, University of Washington, Seattle, WA). The accession codes of the 40 sequences from the NCBI non-redundant database are: NP_000160, NP_038491, CAC44626, XP_318652, AAM29494, XP_315871, NP_611119, AAL87527, XP_235515, NP_000253, 1KTB, NP 506031, NP 822650, NP 624613, AAC99325, NP821803, BAB83765, ZP_00066516, AAM13199, AAP04002, AAG13536, BAC55816, NP_568193, CAC08337, Q42656, BAC66445, T06388, T10860, P14749, AAF04591, BAB12570, NP191190, S45453, P41947, NP 595012, AAG24511, AAB35252, JC5558, NP 811977, and P28351. Sequence identities were calculated without signal sequences in EMBOSS using a Needleman-Wunsch full path matrix algorithm with the BLOSSUM62 matrix, a gap penalty of 10, and a gap extension penalty of 0.5 (Needleman, S. B. & Wunsch, C. D., J Mol Biol 1970, 48:443-53). Least squares superpositions of coordinates were performed using the program LSQMAN (Kleywegt, G. J. & Read, R. J., Structure, 1997, 5:1557-1569) with a distance cutoff of 3.8Å, and coordinate transformations were applied using the program MOLEMAN2 (Kleywegt, G. J. & Read, R. J., Structure, 1997, 5:1557-1569). Molecular figures were prepared using the programs MOLSCRIPT (Kraulis, P. J., J. Appl. Crystallogr., 1991, 24:946-950), BOBSCRIPT (Esnouf, R. M., J. Mol. Graph. Model. 1997, 15:132-34), and GRASP (Nicholls, A., et al., Proteins 1991, 11:281-96). 25

Results

The structure of human α -GAL was determined by x-ray crystallographic methods to a resolution limit of 3.25 Å (see Table 1 below).

Table 1: Crystallographic Statistics

Table 1. Crystallographic Statistics								
Data								
	Native	Ligand						
Beamline	APS 22-ID	APS 22-ID						
Wavelength, Å	1.033	1.033						
Space Group	P3 ₂ 21	P3 ₂ 21						
Cell Lengths, Å	88.5, 88.5, 215.5	90.0, 90.0, 216.5						
Resolution, Å (last shell)	50-3.25 (3.37-3.25)	50-3.45 (3.57-3.45)						
No. of Observations (last shell)	156309 (9921)	91651 (8610)						
No. of Unique Observations (last shell)	16080 (1542)	13922 (1323)						
Completeness, % (last shell)	99.8 (98.7)	99.7 (98.9)						
Multiplicity (last shell)	9.7 (6.5)	6.6 (6.7)						
R _{sym} (last shell)	0.246 (0.740)	0.200 (0.745)						
$\langle 1/\sigma_1 \rangle$ (last shell)	9.1 (2.4)	8.2 (2.4)						
Refinement								
R _{work} / R _{free}	26.2% / 30.1%	28.5% / 32.1%						
No. of Atoms: Protein	6251	6251						
Carbohydrate	268	331						
Other	18	18						
Ramachandran: Favored	74.4%	74.3%						
Allowed	23.0%	23.8%						
Generous	2.5%	1.5%						
Forbidden	0%	0.4%						
RMS Deviations: Bonds	0.009 Å	0.008 Å						
Angles	1.5°	1.5°						
Dihedrals	22.8°	22.8°						
Impropers	0.9°	0.8° .						

 $R_{sym} = \sum_{h} \sum_{i} ||h_{h,i} - \langle h_{h} \rangle| \sum_{h} \sum_{i} ||h_{h,i}|$, where $I_{h,i}$ is the i^{th} intensity measurement of reflection h and $\langle h_{h} \rangle$ is the average intensity of that reflection.

 $R_{work}/R_{irree} = \Sigma_h |F_P - F_C|/\Sigma_h |F_P|$, where F_C is the calculated and F_P is the observed structure factor amplitude of reflection h fo the working/free set, respectively.

The x-ray structure reveals human α -GAL as a homodimeric glycoprotein with each monomer composed of two domains, a $(\beta/\alpha)_8$ domain containing the active site and a C-terminal domain containing eight antiparallel β strands on two sheets in a β sandwich (FIG. 6a). After removal of the 31 residue signal sequence, the first domain extends from residues 32 to 330 and contains the active site formed by the C-terminal ends of the β strands at the center of barrel, a typical location for the active site in $(\beta/\alpha)_8$ domains. The second domain, comprised of residues 331 to 429, packs against the first with an extensive interface, burying 2500 Å² of surface area within one monomer. The dimer has overall protein dimensions of

approximately 75 x 75 x 50Å (FIG. 6b). The molecule is concave in the third dimension and varies in thickness from approximately 20 to 50Å (FIG. 6c). Electron density is visible for 390 and 391 amino acid residues (out of 398 total) in the two copies of the monomer in the crystallographic asymmetric unit; the missing residues occur at the C-terminus. The two monomers pack with an interface that extends the 75Å width of the dimer and buries 2200 Å² of surface area. In the dimer interface, 30 residues from each monomer contribute to the interface, from loops β 1- α 1, β 6- α 6, β 7- α 7, β 8- α 8, β 11- β 12, and β 15- β 16. The dimer is markedly negatively charged, as seen in a surface electrostatic potential (FIG. 6d). With 47 carboxylate groups and only 36 basic residues in the 398 residues in the molecule, the overall charge per monomer is expected to be -11 at neutral pH. The carboxylates are most concentrated around the active site, but in the low pH of the lysosome, many of these groups become protonated, reducing the charge on the molecule. In addition to the negative charges on the protein, the N-linked carbohydrate is highly phosphorylated and sialylated (Lee, K., et al., Glycobiology, 2003, 13:305-13), further increasing its negative electrostatic potential. The N-linked carbohydrates fall distal to the active sites (FIG. 6d). Each monomer contains the three N-linked carbohydrate sites, five disulfide bonds (C52-C94, C56-C63, C142-C172, C202-C223, and C378-C382), two unpaired cysteines (C90 and C174), and three cis prolines (P210, P380, and P389).

As mentioned above, the C-terminal seven and eight residues of each chain have no electron density associated with them and are presumably disordered. This disorder is consistent with the observation of slight heterogeneity in the C-terminus of recombinant human α -GAL, where the truncation of one or two residues from the C-terminus can occur but has no effect upon the activity of the enzyme (Lee, K., et al., *Glycobiology*, 2003, 13:305-13). The structure offers no support for the observation that the removal of 2 to 10 residues from the C-terminus increases the activity of α -GAL (Miyamura, N., et al., *J Clin Invest*, 1996, 98:1809-17), because the final residue seen in the structure falls at least 45Å from each active site and on the opposite face of the molecule.

Substrate specificity and catalytic mechanism

30

In both the native and galactose-soaked crystal structures, electron density appears in the two crystallographically-independent active sites (FIGS. 8a and b). In the galactose-soaked crystal, this density represents α -galactose, the normal catalytic product of the enzyme ($K_i \sim 1 \text{mM}$). In the native structure, this density most likely derives from the

cryoprotectant ethylene glycol, a weak inhibitor of glycoside hydrolases (Tsitsanou, K. E., et al., *Protein Sci*, 1999, 8:741-9), analogous to the insertion of glycerol into carbohydrate binding sites on proteins (Garman, S. C., et al., *Structure*, 2002, 10:425-434; Tsitsanou, K. E., et al., *Protein Sci*, 1999, 8:741-9; Schmidt, A., et al., *Protein Sci*, 1998, 7:2081-8). The two active sites of the dimer are separated by approximately 50 Å. As the enzyme shows little change between the liganded and unliganded structures, there is no evidence for cooperativity between the two sites, although the biochemical evidence is mixed (Dean, K. J. & Sweeley, C. C., *J Biol Chem*, 1979, 254:9994-10000; Bishop, D. F. & Desnick, R. J., *J Biol Chem*, 1981, 256:1307-16).

We have determined that human α -GAL binds α -galactose by making specific contacts to each functional group on the monosaccharide. Residues from seven loops in domain 1 form the *active site*: β 1- α 1, β 2- α 2, β 3- α 3, β 4- α 4, β 5- α 5, β 6- α 6, and β 7- α 7. The active site is formed by the side chains of residues W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267. Thus, a binding pocket defined by the structural coordinates of these amino acids, as set forth in FIG. 1; or a binding pocket whose root mean square deviation from the structure coordinates of the backbone atoms of these amino acids is not more than 1.5 Å is considered a human α -GAL-like binding pocket of this invention. In important embodiments, C172 makes a disulfide bond to C142.

10

20

In the α -GAL/ α -NAGAL family, specificity for the 2 position on the galactose ligand occurs via the β 5- α 5 loop. This was called the "N-acetyl recognition loop" in α -NAGAL (Garman, S. C., et al., *Structure*, 2002, 10:425-434); in the overall α -GAL/ α -NAGAL family "2 position recognition loop" or "2 loop" is appropriate. This loop falls near the boundary of exons 4 and 5 of animal α -GAL/ α -NAGAL, which have a small insertion in this region, resulting in a short helical stretch at the top of the β 5 strand; this insertion is absent in other species. Plant and fungal α -GALs use a Cys and a Trp on this loop to coordinate the 2-hydroxyl on galactose; animal α -GAL uses a Glu and a Leu to recognize the 2-hydroxyl (FIG. 7, green) while animal α -NAGAL uses a Ser and an Ala to recognize an N-acetyl at the 2 position (FIG. 7, yellow). In the animal enzymes, the larger Glu and Leu side chains sterically block the larger N-acetyl substituent, while the smaller Ser and Ala side chains nicely accommodate an N-acetyl group and tolerate a hydroxyl group.

With three different conformations in the 2 loop now identified, the substrate specificity of the other members of the family can be categorized by homology. For

example, genome sequencing of *Drosophila melanogaster* and *Anopheles gambiae* have each identified pairs of genes in the α -GAL family. By examination of the sequences in the 2 loop, two are clearly α -NAGALs while the other two appear to be α -GALs (FIG. 7, yellow and purple). Surprisingly, *Aspergillus niger* contains an enzyme identified as α -GAL that, although only 30% identical to the animal protein sequences, contains a 2 loop virtually identical to animal α -NAGALs (FIG. 7, yellow). We predict this enzyme is primarily an α -NAGAL with partial α -GAL activity, much like human α -NAGAL, which was originally thought to be an α -GAL based upon similar activity (Dean, K. J., et al., *Biochem. Biophys. Res. Commun.*, 1977, 77:1411-7; Schram, A. W., et al., *Biochim. Biophys. Acta*, 1977, 482:138-44).

10

Although human α -GAL makes contacts to each functional group on the α -galactose ligand, the enzyme shows little specificity for the distal portion of the substrate beyond the glycosidic linkage, and the active site cleft is found in a broad opening on the concave surface of the enzyme (FIG. 6c). The lack of substrate specificity of human α -GAL beyond the terminal α -galactose differs slightly from the specificity of other α -GALs, which act only upon substrates containing terminal α 1-6 galactose groups (Kim,W.D., et al., *Phytochemistry*, 2002, 61:621-30). This increased specificity of plant α -GALs may derive from their monomeric structure, as residues buried in the dimer interface of animal α -GALs (e.g., those on the β 1- α 1 loop - Fujimoto, Z., et al., *J Biol Chem*, 2003, 278:20313-8) are available for ligand recognition in monomeric α -GALs.

Both α -GALs and α -NAGALs are α retaining exoglycosidases, where both the substrate and product of the catalytic reactions are α anomers at the 1 position on the galactose ring. This retention of anomeric configuration is accomplished by a double displacement catalytic mechanism where the anomeric carbon undergoes two successive nucleophilic attacks (Vasella, A., et al., *Curr Opin Chem Biol*, 2002, 6:619-29). The two sequential inversions of the anomeric carbon lead to retention of the configuration at the end of the catalytic cycle. In two α -GALs from different species, peptic digestion of covalently trapped intermediates has identified the specific aspartic acid acting as the catalytic nucleophile (Hart, D. O., et al., *Biochemistry*, 2000, 39:9826-36; Ly, H. D., et al., *Carbohydr. Res.*, 2000, 329:539-47). These data, combined with the high resolution structure of chicken α -NAGAL, predict the catalytic mechanism of human α -GAL. In human α -GAL, the first nucleophilic attack upon the substrate comes from D170, cleaving the glycosidic linkage and

leading to a covalent enzyme-intermediate complex. In the second step of the reaction, a water molecule (deprotonated by D231) attacks C1 of the covalent intermediate, liberating the second half of the catalytic product and regenerating the enzyme in its initial state. Human α -GAL operates most efficiently at low pH, consistent with its highly acidic composition and its lysosomal location.

Retaining glycosidases typically have distances of 5-6Å between catalytic carboxylates, while inverting glycosidases typically have distances of 9-11Å between these residues (McCarter, J. D. & Withers, S. G., Curr. Opin. Struct. Biol. 1994, 4:885-92). From these distances, it has been possible to reliably predict the mechanism and function of a glycosidase given its structure. However, this rule must be reconsidered in light of the new structures in the α-GAL/α-NAGAL family: for the known structures in the family, the closest approach of the two catalytic carboxylates is 6.5-7Å, among the largest distances seen for retaining glycosidases.

Comparison to related molecules

15

25

Human α -GAL is most closely related to α -NAGAL, with the human enzymes sharing 49% amino acid sequence identity. A phylogeny tree (FIG. 7) of the 40 proteins most closely related to human α -GAL reveals that vertebrate α -GAL and α -NAGAL cluster and have evolved from a common precursor (Wang, A. M., et al., *J. Biol. Chem.*, 1990, 265:21859-66; Wang, A. M., et al., *Mol. Genet. Metab.*, 1998, 65:165-73), while plant and other α -GALs segregate into distinct clusters. The 40 proteins share from 32 to 78% amino acid sequence identity with human α -GAL, with the sequence conservation higher in domain 1, particularly among residues forming the active site.

The 40 sequences include two structures of a family of 27 glycoside hydrolases: human α -GAL and chicken α -NAGAL (Garman, S. C., et al., *Structure*, 2002, 10:425-434) (51% amino acid identity with human α -GAL). Both enzymes share common tertiary structures: each monomer contains both a $(\beta/\alpha)_8$ N-terminal domain and an antiparallel β C-terminal domain. The N-terminal domains superimpose very well: the chicken α -NAGAL superimposes on the human α -GAL with a root mean square deviation (RMSD) of 0.7Å for 295 C α atoms. Domain 2, with lower sequence conservation, superimposes less well: the chicken domain superimposes on human with an RMSD of 1.3Å for 80 C α atoms. The most important residue in the dimer interface, F273, has 130Å² surface area buried per monomer

upon formation of the dimer. This residue alone (out of the 30 in the dimer interface) accounts for 12% of the buried surface area in the interface. This residue is a Phe or Tyr in most animal α -GALs and α -NAGALs, while in plant α -GALs, the equivalent residue is a Gly. Thus, this residue predicts the dimerization state of the enzyme in different species: Phe or Tyr indicates the enzyme is a dimer, while Gly indicates the enzyme remains a monomer.

N-linked carbohydrate and lysosomal targeting

25

Both endogenous and recombinant α-GAL show a large amount of heterogeneity in the attached carbohydrate, with over 70 different glycoforms (Lee, K., et al., Glycobiology, 2003, 13:305-13; Bishop, D. F. & Desnick, R. J., J Biol Chem, 1981, 256:1307-16; Matsuura, F., et al., Glycobiology, 1998, 8:329-39; LeDonne, N. C., et al., Arch Biochem Biophys, 1983, 224:186-95; Ioannou, Y. A., et al., Biochem J., 1998, 332:789-97). Despite the resolution of the human α-GAL structure, extensive density appears for N-linked carbohydrates. Each monomer has four potential N-linked carbohydrate attachment sites (N139, N192, N215, and N408), the first three of which show carbohydrate electron density. The fourth potential site at N408 contains the amino acid sequence Asn-Pro-Thr, a sequence not ordinarily recognized by the carbohydrate attachment machinery (Gavel, Y. & von Heijne, G., Protein Eng. 1990, 3:433-42), consistent with the absence of carbohydrate at this location in recombinant α -GAL expressed in COS cells (Ioannou, Y. A., et al., Biochem J., 1998, 332:789-97), CHO cells and human cells (Lee, K., et al., Glycobiology, 2003, 13:305-13). The three sites with attached carbohydrate show density in both independent monomers in the asymmetric unit and in both the native and ligand-soaked crystals. Electron density for the carbohydrate attached to N192 is shown in FIG. 9.

The glycosylation pattern differs among the structures in the α -GAL/ α -NAGAL family. The chicken α -NAGAL and human α -GAL each contain three sites, two of which (N192 and N215 in α -GAL numbering) are in common. These two carbohydrates are attached to helices α 4 and α 5, away from the active site and from the dimer interface. The N-linked carbohydrate at N215 is necessary but not sufficient for successful secretion of the active enzyme, and the N192 carbohydrate site improves secretion of the active enzyme (Ioannou, Y. A., et al., *Biochem J.*, 1998, 332:789-97). These two sites have a large proportion of oligomannose-containing carbohydrate, while the N139 site contains no oligomannosyl carbohydrate, only complex carbohydrate (Lee, K., et al., *Glycobiology*, 2003, 13:305-13). Thus the N-linked carbohydrate at N192 and N215 is responsible for targeting

the glycoprotein to the lysosome, because only oligomannosyl carbohydrates contain the lysosomal targeting signal, mannose-6-phosphate (Ghosh, P., et al., Nat Rev Mol Cell Biol, 2003, 4:202-12). The N192 and N215 side chains are 20Å apart on the same face of the molecule, 24 and 23Å away from the active site respectively (FIG. 6d). Unlike many Nlinked carbohydrates that lie along the surface of the protein and shield surface-exposed hydrophobic residues, the carbohydrate at N215 extends away from the protein, in an ideal position to bind to the mannose-6-phosphate receptor (M6PR). Mutation of N215 to Ser eliminates the carbohydrate attachment site, causing inefficient trafficking of the enzyme to the lysosome (Ioannou, Y. A., et al., Biochem J., 1998, 332:789-97) and leading ultimately to the development of Fabry disease (Davies, J. P., et al., Hum Mol Genet, 1993, 2:1051-3). Unique among the carbohydrate attachment sites, N215 shows different primary glycoforms in the two recombinant enzymes used as Fabry disease treatments: in Replagal this site is mostly singly phosphorylated oligomannose, while in Fabrazyme this site is mostly biphosphorylated oligomannose (Lee, K., et al., Glycobiology, 2003, 13:305-13). The M6PR transport pathway is also used by the recombinant glycoprotein in the treatment for Fabry disease: upon injection into the bloodstream of a Fabry patient, the recombinant glycoprotein is delivered into the lysosomes of affected cells via M6PR on the surface. The pharmacological differences between the Replagal and Fabrazyme α-GAL preparations derive from the different glycoforms attached to N192 and N215.

20

25

30

Detailed Description of the Drawings

Figure 1. Atomic structure coordinates of human α-GAL

Figure 1A through 1Z list the atomic structure coordinates for human α -GAL as derived by X-ray diffraction from a crystal of human α -GAL. The following abbreviations are used in FIG. 1: "Atom type" refers to the element whose coordinates are measured. The first letter in the column defines the element.

"X, Y, Z" crystallographically define the atomic position of the element measured.

"OCC" is an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i.e., the same position, in all molecules of the crystal.

"B" is a thermal factor that measures movement of the atom around its atomic center.

Figure 2. Computer Diagram

Computer used to generate a three-dimensional graphical representation of a molecule or molecular complex according to this invention.

- Figure 3. Cross section of a magnetic storage medium.
- Figure 4. Cross section of an optically-readable data storage medium.
- 5 Figure 5. The reaction catalyzed by α -GAL
 - (a) The general reaction of α -GAL. A terminal galactose in the α anomeric configuration is cleaved from an oligosaccharide, glycoprotein, or glycolipid, producing α -galactose (Gal(α 1)) and an alcohol. The carbons are numbered on α -galactose. (b) α -GAL and Fabry disease. The Fabry disease substrate globotriaosylceramide is cleaved by α -GAL to form lactosylceramide. In the absence of the functional enzyme, globotriaosylceramide accumulates in the tissues.

Figure 6. The structure of α-GAL

(a) The α -GAL monomer. The monomer is colored from N (blue) to C terminus (red). Domain 1 contains the active site at the center of the β strands in the $(\beta/\alpha)_8$ barrel, while domain 2 contains antiparallel β strands. The galactose ligand is shown in yellow and red CPK atoms. (b) and (c) Two views of the α -GAL dimer. The ribbon and ligand are colored as in (a). The active sites are 50Å apart in the dimer, on the concave surface of the molecule as viewed from the side in (c). (d) The surface of α -GAL. Two views of the molecular surface are shown with a probe radius of 1.4Å, with the electrostatic surface potential plotted from – 10kT (red) to +10kT (blue). The N-linked carbohydrate is shown in green and is not included in the surface potential calculation. The orientation at left is similar to (b).

Figure 7. Evolutionary relationships in the α -GAL/ α -NAGAL family

A phylogeny tree demonstrates the relationships of 40 sequences most closely related to human α -GAL. The length of the line connecting each name represents the distance between the two sequences. The sequences above the black line have an insertion creating a turn of helix in the β 5/ α 5 loop, while the lower sequences lack this insertion. α -NAGALs are in yellow, while α -GALs are in green, blue and purple.

Figure 8. The active site of \alpha-GAL

(a) and (b) Electron density in human α -GAL from native and galactose-soaked crystals. The electron density is shown in stereo contoured at 1.1 σ from a σ_A -weighted simulated annealing composite omit map, with side chains from active site residues colored as in fig 6. The red density does not derive from the protein and is interpreted as an ethylene glycol

molecule in (a) and the catalytic product galactose in (b). In (c) the superimposed active sites of human α -GAL (green), and chicken α -NAGAL (yellow) are shown in stereo. The β 5- α 5 loop that differs among the two structures appears at lower right.

Figure 9. N-linked carbohydrate

The N-linked carbohydrate attached to N192 is shown with helix α4. Electron density from a σ_A-weighted simulated annealing composite omit map (grey) is contoured at 1.1σ. Five sugar residues have been built into the electron density at this site.

Figure 10. The active site of α -GAL

A schematic representation of the human α -GAL active site with a galactose molecule buried within.

Equivalents

10

15

Those skilled in the art will recognize, or be able to ascertain using no more than routine experimentation, many equivalents to the specific embodiments of the invention described herein. Such equivalents are intended to be encompassed by the following claims.

All references disclosed herein are incorporated by reference in their entirety. What is claimed is presented below and is followed by a Sequence Listing.

We claim:

Claims

- 1. A computer for producing a three-dimensional representation of:
 - a. a molecule or molecular complex, wherein said molecule or molecular complex comprises a binding pocket defined by structure coordinates of human α-galactosidase amino acids W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1; or
 - b. a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, wherein said computer comprises:
- (i) a computer-readable data storage medium comprising a data storage material encoded with computer-readable data, wherein said data comprises the structure coordinates of human α-galactosidase amino acids W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1;
- (ii) a working memory for storing instructions for processing said computer-readable data;
- (iii) a central-processing unit coupled to said working memory and to said computerreadable data storage medium for processing said computer-machine readable data into said three-dimensional representation; and
- (iv) a display coupled to said central-processing unit for displaying said threedimensional representation.
- 2. The computer according to claim 1, wherein the computer produces a three-dimensional representation of:
- a. a molecule or molecular complex defined by structure coordinates of all of the human α -galactosidase amino acids set forth in FIG. 1, or

b. a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å; and

wherein said computer readable data contains the coordinates of all of the human α -galactosidase amino acids set forth in FIG. 1.

- 3. A computer for determining at least a portion of the structure coordinates corresponding to X-ray diffraction data obtained from a molecule or molecular complex, wherein said computer comprises:
- (a) a computer-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structural coordinates of human α -galactosidase according to FIG. 1;
- (b) a computer-readable data storage medium comprising a data storage material encoded with computer-readable data, wherein said data comprises X-ray diffraction data obtained from said molecule or molecular complex;
- (c) a working memory for storing instructions for processing said computer-readable data of (a) and (b);
- (d) a central-processing unit coupled to said working memory and to said computerreadable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said computer-readable data of (b) into structure coordinates; and
- (e) a display coupled to said central-processing unit for displaying said structure coordinates of said molecule or molecular complex.
- 4. The computer according to claim 3, wherein said molecule or molecular complex comprises a polypeptide having α-galactosidase activity.

- 5. A method for evaluating the potential of a chemical entity to associate with:
- a) a molecule or molecular complex comprising a binding pocket defined by structure coordinates of human α-galactosidase amino acids W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1, or
- b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å comprising the steps of:
- i) employing computational means to perform a fitting operation between the chemical entity and a binding pocket defined by structure coordinates of human α-galactosidase amino acids W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å; and
- ii) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket.
- 6. The method according to claim 5, wherein the method evaluates the potential of a chemical entity to associate with:
- a. defined by structure coordinates of all of the human α -galactosidase amino acids, as set forth in FIG. 1, or
- b. a homologue of said molecule or molecular complex having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.
- 7. A method for identifying a potential agonist or antagonist of a molecule comprising a human α-galactosidase domain 1-like binding pocket comprising the steps of:
- a. using the atomic coordinates of W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1 ± a root mean square

deviation from the backbone atoms of said amino acids of not more than 1.5 Å, to generate a three-dimensional structure of molecule comprising a human α -galactosidase domain 1-like binding pocket;

- b. employing said three-dimensional structure to design or select said potential agonist or antagonist;
 - c. synthesizing said agonist or antagonist; and
- d. contacting said agonist or antagonist with said molecule to determine the ability of said potential agonist or antagonist to interact with said molecule.
- 8. The method according to claim 7, wherein in step a., the atomic coordinates of all the amino acids of human α -galactosidase according to FIG. 1 \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å are used.

Abstract

This invention pertains to the X-ray crystal structure of the human α -galactosidase glycoprotein. More specifically, the invention relates to crystallized compositions of human α -galactosidase and to crystallized complexes of human α -galactosidase and its catalytic product α -galactose. The invention further relates to a computer programmed with the structure coordinates of the human α -galactosidase's active site wherein said computer is capable of displaying a three-dimensional representation of that active site. The invention also relates to methods for rational drug design based on the structural data for human α -galactosidase provided on computer readable media, as analyzed on a computer system having suitable computer algorithms.

FIGURE 1

HUMAN Q-GALACTOSIDASE COORDINATES

CHAIN A								
		Atom Type	Resid	£	x	Y <u>Z</u>	0СС В	
MOTA	1	N	LEU A	32	-14.824	53.775 124.809	1.00 67.49	N
ATOM	2	CA	LEU A	32	-16.090	53.328 125.458	1.00 67.86	C
ATOM ATOM	3	C	LEU A LEU A	32 32	-15.906 -15.672	51.947 126.081 50.968 125.380	1.00 66.10 1.00 67.72	C
MOTA	5	СВ	LEU A	32	-17.218	53.293 124.425	1.00 37.72	č
MOTA	6	CG	LEU A	32	-18.563	52.754 124.909	1.00 76.53	Ċ
MOTA	7		LEU A	32	-19.013	53.542 126.120	1.00 82.27	C
ATOM	8		LEU A	32	-19.587	52.849 123.798	1.00 75.72	C
ATOM ATOM	9 10	N CA	ASP A ASP A	33 33	-16.010 -15.833	51.872 127.402 50.609 128.110	1.00 62.63 1.00 66.42	N C
ATOM	11	c	ASP A	33	-17.078	49.732 128.061	1.00 66.28	č
MOTA	12	Õ	ASP A	33	-17.847	49.662 129.010	1.00 70.72	0
MOTA	13	СВ	ASP A	33	-15.429	50.886 129.565	1.00 76.45	c
MOTA	14 15	CG	ASP A	33 33	-15.213 -16.204	49.613 130.376 48.914 130.682	1.00 89.48 1.00 92.42	C O
ATOM ATOM	16		ASP A	33	-14.045	49.310 130.710	1.00101.27	ő
ATOM	17	N	ASN A	34	-17.268	49.065 126.934	1.00 63.97	N
MOTA	18	CA	ASN A	34	-18.403	48.178 126.733	1.00 58.89	C
ATOM	19	C	ASN A	34	-17.827	46.786 126.543	1.00 58.39	C
ATOM ATOM	20 21	O CB	ASN A ASN A	34 34	-18.512 -19.157	45.868 126.086 48.579 125.474	1.00 59.56 1.00 50.46	0 C
MOTA	22	CG	ASN A	34	-18.228	48.774 124.289	1.00 44.58	č
MOTA	23	OD1	ASN A	34	-17.200	48.106 124.184	1.00 48.14	0
MOTA	24		ASN A	34	-18.584	49.689 123.390	1.00 32.72	N
ATOM ATOM	·25 26	N CA	GLY A	35 35	-16.552 -15.885	46.648 126.892 45.374 126.748	1.00 55.86 1.00 53.67	N C
MOTA	27	C	GLY A	35	-15.709	45.048 125.278	1.00 52.92	č
ATOM	28	ō	GLY A	35	-15.539	43.886 124.908	1.00 57.86	0
ATOM	29	N	LEU A	36	-15.758	46.071 124.430	1.00 47.94	N
MOTA	30 31	C A	LEU A	36 36	-15.579 -14.389	45.871 122.994 46.650 122.493	1.00 46.06 1.00 46.43	C C
ATOM ATOM	32	Ö	LEU A	36	-14.042	47.703 123.039	1.00 47.09	ō
ATOM	33	ČВ	LEU A	36	-16.812	46.304 122.206	1.00 51.34	С
MOTA	34	CG	LEU A	36	-18.046	45.428 122.366	1.00 52.68	c
MOTA	35		LEU A	36	-19.072	45.835 121.327 43.965 122.205	1.00 57.25 1.00 56.03	C C
ATOM ATOM	36 37	N N	LEU A ALA A	36 37	-17.668 -13.770	46.135 121.440	1.00 46.90	N
MOTA	38	CA	ALA A	37	-12.610	46.789 120.883	1.00 49.14	С
MOTA	39	С	ALA A	37	-11.562	46.863 121.973	1.00 49.54	C
ATOM	40	0	ALA A	37	-11.079	47.946 122.303	1.00 48.93	0 C
ATOM ATOM	41 42	CB N	ALA A ARG A	37 38	-12.971 -11.245	48.179 120.416 45.710 122.559	1.00 55.24 1.00 51.16	N
ATOM	43	CA	ARG A	38	-10.220	45.658 123.598	1.00 58.37	ë
MOTA	44	С	ARG A	38	-8.943	45.500 122.802	1.00 54.73	С
ATOM	45	0	ARG A	38	-7.864	45.256 123.342	1.00 61.96	0
ATOM ATOM	46 47	CB CG	ARG A	38 38	-10.388 -11.755	44.457 124.538 44.326 125.213	1.00 64.33 1.00 66.46	C C
ATOM	48	CD	ARG A	38	-12.329	45.665 125.696	1.00 68.63	č
ATOM	49	NE	ARG A	38	-11.542	46.310 126.743	1.00 65.38	N
MOTA	50	CZ	ARG A	38	-11.845	47.494 127.264	1.00 70.22	C
ATOM ATOM	51 52		ARG A	38 38	-12.915 -11.078	48.153 126.835 48.025 128.205	1.00 66.18 1.00 76.54	N N
ATOM	53	N	THR A	39	-9.114	45.629 121.492	1.00 42.63	N
MOTA	54	CA	THR A	39	-8.041	45.553 120.513	1.00 39.39	С
MOTA	55	C	THR A	39	-8.555	46.298 119.290	1.00 38.04	C
MOTA MOTA	56 57	O CB	THR A	39 39	-9.753 -7.741	46.284 119.008 44.105 120.101	1.00 40.98 1.00 31.04	0 C
ATOM	58		THR A	39	-8.932	43.513 119.570	1.00 43.60	ŏ
MOTA	59		THR A	39	-7.270	43.292 121.283	1.00 29.17	С
ATOM	60	N	PRO A	40	-7.661	46.968 118.555	1.00 38.37	N
MOTA MOTA	61 62	CA	PRO A	40 40	-8.115 -9.048	47.696 117.367 46.806 116.520	1.00 38.65 1.00 36.72	C C
MOTA	63	ŏ	PRO A	40	-8.684	45.685 116.166	1.00 50.49	0
ATOM	64	CB	PRO A	40	-6.803	48.032 116.658	1.00 42.95	С
MOTA	65	CG	PRO A	40	-5.827	48.173 117.806	1.00 44.34	Ċ
MOTA MOTA	66 67	CD N	PRO A THR A	40 41	-6.194 -10.254	47.019 118.696 47.294 116.219	1.00 44.72 1.00 30.56	C N
MOTA	68	CA	THR A	41	-11.235	46.536 115.417	1.00 22.13	č
MOTA	69	С	THR A	41	-10.684	46.192 114.045	1.00 21.75	С
ATOM	70	0	THR A	41	-10.020	47.020 113.423 47.347 115.152	1.00 17.46	0
ATOM ATOM	71 72	CB OG1	THR A	41 41	-12.506 -12.901	48.035 116.348	1.00 18.74 1.00 29.21	C
0.1	. 4	561	A	••	12.701	110.340		J

MOTA	73	CG2	THR	A 41	-13.626	46.428	114.666	1.00 3.31	С
MOTA	74	N		A 42	-10.967	44.987	113.561	1.00 27.61	N
MOTA	75	CA		A 42	-10.486		112.234	1.00 31.65	С
MOTA	76	C		A 42	-11.646		111.330	1.00 32.03	Ç
ATOM	77	0		A 42	-12.479		111.701	1.00 37.57	0
MOTA MOTA	78 79	CB		A 42	-9.539		112.342	1.00 37.02	C
MOTA	80	SD	MET	A 42 A 42	-8.362 -7.217		113.237	1.00 32.14	C S
MOTA	81	CE	MET		-6.528		113.180 111.547	1.00 27.50 1.00 31.36	Ċ
MOTA	82	N	GLY		-11.696		110.144	1.00 19.78	N
MOTA	83	CA	GLY		-12.767		109.215	1.00 24.08	Ċ
MOTA	84	С	GLY		-12.606		107.848	1.00 26.38	Ċ
MOTA	85	0	GLY	A 43	-11.502		107.434	1.00 35.82	0
MOTA	86	N	TRP		-13.725		107.145	1.00 20.58	N
MOTA	87	CA	TRP		-13.751		105.799	1.00 18.47	C
MOTA	88	C	TRP		-14.863		105.710	1.00 19.26	C
MOTA	89 90	0	TRP		-15.935		106.301	1.00 22.29	0 C
MOTA MOTA	91	CB CG	TRP		-14.015 -13.961		104.763	1.00 13.98 1.00 28.86	c
MOTA	92		TRP		-12.841		103.520	1.00 43.13	Č
ATOM	93		TRP		-15.074		102.465	1.00 29.85	č
ATOM	94			A 44	-13.186		101.265	1.00 44.22	N
MOTA	95			A 44	-14.550		101.187	1.00 38.52	С
MOTA	96	CE3	TRP	A 44	-16.461	45.524	102.653	1.00 19.33	С
MOTA	97		TRP		-15.367		100.102	1.00 39.43	Č
MOTA	98		TRP		-17.274		101.576	1.00 28.01	c
MOTA	99			A 44	-16.723		100.318	1.00 40.64	C
ATOM	100	N	LEU		-14.609 -15.583		104.951 104.806	1.00 15.68 1.00 8.20	N C
MOTA MOTA	101 102	CA C	LEU		-15.575		103.344	1.00 8.64	Ċ
ATOM	103	ŏ	LEU		-14.552		102.779	1.00 5.90	õ
ATOM	104	ĊВ	LEU		-15.198		105.694	1.00 3.31	Ċ
ATOM	105	CG	LEU		-16.294		106.050	1.00 5.81	C
ATOM	106		LEU		-15.648		106.684	1.00 12.88	С
MOTA	107		LEU		-17.052		104.820	1.00 21.03	C
ATOM	108	N	HIS		-16.745		102.744	1.00 3.31	N
MOTA	109	CA	HIS		-16.919		101.340	1.00 11.17	C
MOTA	110	C	HIS HIS		-16.579 -16.281	50.976	100.856 99.675	1.00 21.93 1.00 29.71	C O
MOTA ATOM	111 112	O CB	HIS		-18.364		100.942	1.00 23.71	Č
ATOM	113	CG	HIS		-19.281		101.003	1.00 28.93	č
MOTA	114		HIS		-19.351	51.374	99.996	1.00 35.79	N
ATOM	115		HIS		-20.150		101.958	1.00 28.46	С
ATOM	116	CE1	HIS	A 46	-20.224	52.309	100.328	1.00 32.31	С
MOTA	117	NE2	HIS		-20.723		101.514	1.00 19.72	N
ATOM	118	N	TRP		-16.598		101.733	1.00 19.43	N
ATOM	119	CA		A 47	-16.373		101.260	1.00 18.18	C C
MOTA	120	C O	TRP		-15.325 -15.664	53.759	100.182	1.00 19.31 1.00 17.77	0
ATOM ATOM	121 122	СВ	TRP TRP	A 47	-16.176		102.419	1.00 23.78	č
ATOM	123	CG		A 47	-16.419		101.936	1.00 38.36	č
ATOM	124		TRP		-15.536		101.925	1.00 46.06	С
ATOM	125	CD2	TRP	A 47	-17.605	56.208	101.287	1.00 40.43	С
MOTA	126	NE1	TRP	A 47	-16.096		101.302	1.00 47.00	N
MOTA	127			A 47	-17.367		100.901	1.00 44.04	C
MOTA	128	CE3		A 47	-18.847		100.991	1.00 40.44	C C
MOTA	129		TRP		-18.323		100.235	1.00 45.58	c
ATOM ATOM	130 131		TRP TRP		-19.797 -19.528	57.721	100.329 99.958	1.00 44.04	c
MOTA	132	N	GLU		-14.068		100.568	1.00 13.66	Ñ
ATOM	133	CA	GLU		-13.046	54.186	99.590	1.00 6.43	C
ATOM	134	C	GLU		-13.071	53.427	98.260	1.00 5.74	С
ATOM	135	0	GLU	A 48	-12.909	54.026	97.206	1.00 7.32	0
ATOM	136	CB	GLU		-11.640		100.210	1.00 3.31	C
MOTA	137	CG	GLU		-10.500	54.771	99.396	1.00 10.31	C
MOTA	138	CD	GLU		-10.188	54.109	98.042	1.00 23.63	C C
ATOM ATOM	139 140		GLU		-9.778 -10.342	52.930 54.773	98.018 96.996	1.00 28.74 1.00 34.69	Ö
ATOM	141	N N	ARG		-13.279	52.119	98.302	1.00 34.69	N
ATOM	142	CA	ARG		-13.258	51.319	97.085	1.00 18.71	С
ATOM	143	Ċ	ARG		-14.505	51.367	96.218	1.00 23.25	С
MOTA	144	0	ARG	A 49	-14.441	51.101	95.016	1.00 23.40	0
MOTA	145	CB	ARG		-12.947	49.865	97.440	1.00 28.83	C
ATOM	146	CG	ARG		-12.685	48.983	96.244	1.00 33.89	c
ATOM	147	CD	ARG		-11.610	49.585	95.354	1.00 50.93	C N
MOTA MOTA	148 149	NE CZ	ARG		-11.077 -11.745	48.596 48.111	94.424 93.385	1.00 62.30 1.00 65.06	C
ATOM	150		ARG ARG		-12.977	48.537	93.130	1.00 53.00	N
MOTA	151		ARG		-11.193	47.173	92.623	1.00 68.57	N
ATOM	152	N	PHE		-15.633	51.721	96.819	1.00 18.53	N
MOTA	153	CA	PHE		-16.885	51.752	96.083	1.00 19.91	С

		_						06 050	1 00 25	70	С	
	154	С	PHE A				3.015		1.00 25.			
ATOM	155	0	PHE A	A 5	0 -18.7	149 5	53.184		1.00 30.		0	
ATOM	156	CB	PHE A	A 51	-17.6	594 5	50.526	96.479	1.00 3.	. 31	С	
MOTA	157	CG	PHE A	A 5	0 -17.0	37 4	19.234	96.080	1.00 3.	. 31	C	
	158		PHE .				18.700	94.796	1.00 7.	.11	C	
	159		PHE				18.575			. 31	С	
	160		PHE				17.530			31	С	
										31	č	
	161		PHE A				17.397					
	162	CZ	PHE A				16.877			. 31	C	
ATOM	163	N	MET .	A 5	1 -17.2	256 5	53.908	97.113	1.00 30.	. 81	N	
MOTA	164	CA	MET .	A 5	1 -17.9	967 5	55.151	97.352	1.00 35.	. 74	С	
	165	С	MET .	A 5	1 -19.4	174	54.972	97.329	1.00 38.	.71	С	
	166	õ	MET .				3.965		1.00 44		0	
	167	ČВ	MET .				56.181		1.00 32		Ċ	
									1.00 40		č	
_	168	CG	MET .				56.360					
	169	SD	MET .				57.763		1.00 60		S	
ATOM	170	CE	MET .	A 5	1 -15.	519 5	58.994		1.00 60		С	
ATOM	171	N	CYS .	A 5	2 -20.1	162 5	55.956	96.766	1.00 43.	. 24	N	
	172	CA	CYS .	A 5	2 -21.6	511 9	55.932	96.714	1.00 50	. 44	C	
	173	С	CYS .				55.641		1.00 52	. 54	C	
	174	ō	CYS .				56.497		1.00 51		0	
								97.189	1.00 53		č	
ATOM	175	CB	CYS .				57.276				Š	
	176	SG	CYS .				57.393		1.00 59			
ATOM	177	N	ASN .	A 5			54.417		1.00 56		N	
ATOM	178	CA	ASN .	A 5	3 -22.3	252 9	53.988	93.541	1.00 56	. 33	C	
MOTA	179	С	ASN .	A 5	3 -23.0	563 5	53.399	93.537	1.00 54	. 88	С	
ATOM	180	ō	ASN				52.474	94.291	1.00 51		0	
ATOM	181	СВ	ASN				52.952	93.030	1.00 59		С	
							52.516	91.631	1.00 58		č	
MOTA	182	CG	ASN .						1.00 59		Ö	
MOTA	183		ASN				52.053	91.342				
ATOM	184	NDS	ASN	A 5			52.655	90.745	1.00 60		N	
MOTA	185	N	LEU	A 5	4 -24.	532 9	53.913	92.675	1.00 57		N	
MOTA	186	CA	LEU	A 5	4 -25.	901 9	53.418	92.637	1.00 61	. 04	С	
ATOM	187	С	LEU		4 -26.	378	52.881	91.292	1.00 69	. 48	С	
ATOM	188	ŏ	LEU				52.226	91.220	1.00 71	. 14	0	
	189	СВ	LEU				54.518	93.084	1.00 52		Ċ	
ATOM								94.490	1.00 47		č	
MOTA	190	CG	LEU				55.089					
MOTA	191		LEU				55.905	94.578	1.00 51		C	
ATOM	192	CD2	LEU	A 5			55.958	94.805	1.00 44		С	
ATOM	193	N	ASP	A 5	5 -25.	622	53.152	90.233	1.00 78	. 93	N	
MOTA	194	CA	ASP	A 5	5 -25.	995	52.715	88.884	1.00 80	. 51	C	
ATOM	195	C		A 5			51.206	88.701	1.00 76	. 75	C	
ATOM	196	ŏ		5			50.731	88.079	1.00 76		0	
								87.849	1.00 88		č	
MOTA	197	CB		A 5			53.451					
MOTA	198	CG		A 5			53.369	86.445	1.00 92		C	
MOTA	199	OD1		A 5			53.916	85.523	1.00 96		0	
MOTA	200	OD2	ASP	A 5	5 -26.	775	52.766	86.262	1.00 89	. 47	0	
ATOM	201	N	CYS	A 5	6 -26.	815	50.456	89.230	1.00 76	. 43	N	
ATOM	202	CA	CYS			774	49.010	89.130	1.00 83	. 63	C	
ATOM	203	Ċ	CYS		6 -27.		48.562	87.754	1.00 88	. 30	С	
	204		CYS		6 -27.		47.395	87.521	1.00 90		ō	
ATOM		0							1.00 87		č	
MOTA	205	СВ	CYS		6 -27.		48.416	90.242				
ATOM	206	SG	CYS		6 -27.		49.183	91.844	1.00100		S	
ATOM	207	N	GLN	A 5	7 -27.	244	49.512	86.833	1.00 95	. 89	N	
MOTA	208	CA	GLN	A 5	7 -27.	620	49.239	85.460	1.00105	. 09	С	
ATOM	209	С	GLN		7 -26.	373	48.907	84.654	1.00107	.10	С	
ATOM	210	0	GLN		7 -26.		47.750	84.300	1.00106	. 26	0	
ATOM	211	ČВ	GLN		7 -28.		50.454	84.859	1.00111	. 37	С	
MOTA	212	CG	GLN		7 -29.		50.532	85.205	1.00117		č	
									1.00121		č	
ATOM	213	CD	GLN		7 -30.		49.342	84.666			ō	
ATOM	214		GLN		7 -30.		49.098	83.458	1.00121			
MOTA	215	NE2	GLN		7 -31.		48.585	85.560	1.00120		N	
ATOM	216	N	GLU	A 5	8 -25.	568	49.929	84.374	1.00107		N	
MOTA	217	CA	GLU	A 5	8 -24.	341	49.763	83.602	1.00102		C	
ATOM	218	С	GLU		8 -23.	168	49.325	84.469	1.00 92	. 49	С	
ATOM	219	Ō	GLU		8 -22.		48.962	83.968	1.00 97	. 97	0	
ATOM	220	СВ	GLU		8 -23.		51.069	82.873	1.00106		C	
							51.375	81.703	1.00115		Č	
MOTA	221	CG	GLU				52.688	81.015	1.00113		č	
ATOM	222	CD	GLU		8 -24.	-					0	
ATOM	223		GLU		8 -24.		53.751	81.646	1.00127			
ATOM	224	OE2	GLU		8 -24.		52.654	79.840	1.00126		0	
ATOM	225	N	GLU	A 5	9 -23.		49.354	85.776	1.00 77		N	
ATOM	226	CA	GLU		9 -22.		48.960	86.707	1.00 71	. 10	С	
ATOM	227	C	GLU		9 -23.		48.298	87.890	1.00 64		С	
ATOM	228	ŏ	GLU		9 -23.		48.926	88.913	1.00 66		Ó	
ATOM	229	СВ	GLU		9 -21.		50.188	87.145	1.00 79		č	
	230	CG					50.696	86.081	1.00 96		č	
MOTA			GLU				52.212		1.00106		Č	
ATOM	231	CD	GLU		9 -20.			85.968				
MOTA	232		GLU		9 -20.		52.891	87.019	1.00111		0	
ATOM	233		GLU		9 -20.		52.725	84.826	1.00111		0	
MOTA	234	N	PRO	A 6	0 -23.	326	47.010	87.749	1.00 60	. U6	N	

ATOM	235	CA	PRO A	60	-23.982	46.169	88.754	1.00 63.63	С
ATOM	236	c	PRO A	60	-23.031	45.545	89.774	1.00 67.46	č
ATOM	237	ŏ	PRO A	60	-23.459	45.035	90.819	1.00 63.91	ō
ATOM	238	CB	PRO A	60	-24.661	45.112	87.903	1.00 62.40	Ċ
MOTA	239	CG	PRO A	60	-23.633	44.894	86.838	1.00 56.39	С
MOTA	240	CD	PRO A	60	-23.238	46.303	86.459	1.00 58.46	С
MOTA	241	N	ASP A	61	-21.740	45.585	89.469	1.00 70.71	N
MOTA	242	CA	ASP A	61	-20.746	44.999	90.357	1.00 71.23	С
MOTA	243	C	ASP A	61	-20.074	45.989	91.298	1.00 65.01	Ç
MOTA	244	0	ASP A	61	-19.496	45.586	92.299	1.00 60.40	o
MOTA	245	CB	ASP A	61	-19.690	44.268	89.528	1.00 82.26	c
ATOM	246	CG	ASP A	61	-20.283	43.147	88.695	1.00 89.82	C
MOTA	247		ASP A	61	-20.865	42.211	89.288	1.00 86.48	0
MOTA	248	OD3		61	-20.169	43.204 47.275	87.450 90.977	1.00 94.31 1.00 61.91	0
MOTA	249	N	SER A	62 62	-20.137 -19.533	48.294	91.825	1.00 55.96	, C
MOTA MOTA	250 251	CA C	SER A	62	-20.657	48.915	92.641	1.00 48.78	, ,
MOTA	252	Ö	SER A	62	-20.439	49.606	93.629	1.00 48.50	ŏ
ATOM	253	СB	SER A	62	-18.843	49.338	90.954	1.00 62.78	č
ATOM	254	OG	SER A	62	-17.958	48.701	90.047	1.00 64.54	ŏ
ATOM	255	N	CYS A	63	-21.867	48.635	92.181	1.00 36.06	N
ATOM	256	CA	CYS A	63	-23.117	49.070	92.776	1.00 32.68	С
MOTA	257	С	CYS A	63	-23.243	48.574	94.216	1.00 26.28	С
MOTA	258	0	CYS A	63	-22.960	47.419	94.512	1.00 40.86	0
MOTA	259	CB	CYS A	63	-24.244	48.530	91.897	1.00 50.02	С
MOTA	260	SG	CYS A	63	-25.788	47.955	92.660	1.00 84.72	S
MOTA	261	N	ILE A	64	-23.669	49.460	95.108	1.00 17.87	Ŋ
MOTA	262	CA	ILE A	64	-23.841	49.138	96.518	1.00 16.03	C
ATOM	263	C	ILE A	64	-25.138	48.357	96.796	1.00 23.75	c
MOTA	264	0	ILE A	64	-26.206	48.950	96.977	1.00 26.05	O C
MOTA	265 266	CB	ILE A	64 64	-23.856 -22.539	50.427 51.180	97.358 97.179	1.00 11.27 1.00 15.20	Č
MOTA MOTA	267		ILE A	64	-24.095	50.090	98.813	1.00 14.96	č
ATOM	268		ILE A	64	-22.486	52.490	97.923	1.00 33.05	č
ATOM	269	N	SER A	65	-25.038	47.029	96.852	1.00 29.07	Ň
ATOM	270	CA	SER A	65	-26.207	46.182	97.095	1.00 35.48	Ċ
ATOM	271	Č.	SER A	65	-25.910	44.988	97.987	1.00 39.53	č
ATOM	272	ō	SER A	. 65	-24.763	44.549	98.102	1.00 46.31	· 0
ATOM	273	СВ	SER A	65	-26.725	45.623	95.786	1.00 42.49	С
MOTA	274	OG	SER A	65	-26.003	44.448	95.475	1.00 57.55	0
ATOM	275	N	GLU A	66	-26.964	44.432	98.579	1.00 46.25	N
ATOM	276	CA	GLU A	66	-26.808	43.265	99.442	1.00 51.68	С
MOTA	277	С	GLU A	66	-26.093	42.193	98.639	1.00 49.33	C
MOTA	278	0	GLU A	66	-25.391	41.340	99.185	1.00 48.58	0
MOTA	279	CB	GLU A	66	-28.172	42.753	99.939	1.00 52.13	C
MOTA	280	CG	GLU A	66	-29.251	42.627	98.884	1.00 60.06	C
MOTA	281	CD	GLU A	66	-30.427	41.805	99.368	1.00 66.09	c
MOTA	282		GLU A	66	-30.263	40.579	99.520	1.00 60.99	0 0
ATOM	283		GLU A LYS A	66 67	-31.510 -26.263	42.378 42.263	99.611 97.325	1.00 70.88 1.00 50.35	N
MOTA MOTA	284 285	N CA	LYS A LYS A	67	-25.616	41.319	96.441	1.00 59.16	Č
ATOM	286	C	LYS A	67	-24.120	41.573	96.569	1.00 50.62	č
ATOM	287	ŏ	LYS A	67	-23.341	40.637	96.721	1.00 57.82	ŏ
ATOM	288	СВ	LYS A	67	-26.108	41.524	95.007	1.00 76.41	č
ATOM	289	CG	LYS A	67	-27.591	41.155	94.806	1.00 93.54	С
ATOM	290	CD	LYS A	67	-28.450	42.296	94.217	1.00102.67	C
ATOM	291	CE	LYS A	67	-27.959	42.782	92.844	1.00103.90	С
MOTA	292	NZ	LYS A	67	-27.807	41.690	91.845	1.00 98.42	N
MOTA	293	N	LEU A	68	-23.719	42.839	96.543	1.00 41.00	N
MOTA	294	CA	LEU A	68	-22.304	43.169	96.681	1.00 35.92	C
MOTA	295	C	LEU A	68	-21.710	42.564	97.957	1.00 28.69	C
MOTA	296	0	LEU A	68	-20.907	41.628	97.913	1.00 30.00	0
ATOM	297	CB	LEU A	68	-22.109	44.691	96.683	1.00 37.88	c c
MOTA	298	CG	LEU A	68	-20.742 -19.593	45.295	97.056 96.493	1.00 30.06 1.00 32.82	Ċ
MOTA	299		LEU A	68	-19.593	44.472 46.722	96.528	1.00 32.82	Ċ
MOTA MOTA	300 301	N N	LEU A PHE A	68 69	-20.684	43.100	99.099	1.00 33.04	N
ATOM	302	CA	PHE A	69	-21.599		100.374	1.00 29.31	Ċ
ATOM	303	C	PHE A	69	-21.635	41.071		1.00 35.20	ċ
ATOM	304	ŏ	PHE A	69	-20.617	40.426		1.00 35.73	ō
MOTA	305	СВ	PHE A	69	-22.413		101.519	1.00 26.29	С
ATOM	306	ĊĠ	PHE A	69	-22.200		101.698	1.00 26.15	С
MOTA	307		PHE A	69	-21.182	45.145	102.522	1.00 24.44	С
MOTA	308	CD2	PHE A	69	-23.007		101.032	1.00 28.73	c c
MOTA	309		PHE A	69	-20.973		102.682	1.00 27.34	ç
MOTA	310		PHE A	69	-22.804		101.187	1.00 23.88	c
MOTA	311	CZ	PHE A	69	-21.786		102.015	1.00 25.71	C
MOTA	312	N	MET A	70	-22.825		100.240	1.00 43.20	N C
MOTA	313	CA	MET A	70 70	-23.073		100.287 99.626	1.00 47.28 1.00 46.42	c
MOTA MOTA	314 315	С 0	MET A	70 70	-21.931 -21.475	38.329 37.287	100.107	1.00 49.69	Ö
VIOU.	313	U	MET A	, 0	-21.4/3	31.201		1.00 47.07	J

		an	~~				_
MOTA	316	CB MET A	70	-24.379	38.755 99.563	1.00 43.22	c
ATOM	317 318	CG MET A	70 70	-24.925	37.381 99.864	1.00 46.78	C S
MOTA MOTA	319	CE MET A	70	-26.352 -27.493	36.950 98.839 38.341 99.190	1.00 70.05 1.00 58.66	Č
ATOM	320	N GLU A	71	-21.479	38.872 98.505	1.00 43.02	Ŋ
ATOM	321	CA GLU A	71	-20.379	38.282 97.768	1.00 43.81	Ċ
ATOM	322	C GLU A	71	-19.153	38.421 98.664	1.00 42.37	Č
MOTA	323	O GLU A	71	-18.559	37.431 99.095	1.00 46.48	C
MOTA	324	CB GLU A	71	-20.185	39.040 96.454	1.00 52.02	c c
MOTA	325	CG GLU A	71	-19.343	38.314 95.414	1.00 61.53	С
MOTA	326	CD GLU A	71	-19.348	39.006 94.047	1.00 67.25	Ċ
MOTA	327	OE1 GLU A	71	-18.665	38.503 93.127	1.00 69.17	0
MOTA	328	OE2 GLU A	71	-20.034	40.045 93.889	1.00 60.67	0
ATOM	329	N MET A	72	-18.799	39.666 98.952	1.00 39.30	N C
ATOM	330	CA MET A	72 72	-17.669 -17.607	39.969 99.807	1.00 40.60 1.00 47.07	c
ATOM ATOM	331 332	C MET A	72	-16.578	39.067 101.042 38.441 101.298	1.00 47.07	Č
ATOM	333	CB MET A	72	-17.747	41.430 100.226	1.00 37.04	č
ATOM	334	CG MET A	72	-17.390	42.385 99.113	1.00 20.85	č
ATOM	335	SD MET A	72	-15.643	42.198 98.762	1.00 34.40	S
ATOM	336	CE MET A	72	-15.552	42.658 97.119	1.00 3.31	0 C C S
ATOM	337	N ALA A	73	-18.704	39.004 101.799	1.00 51.91	N
ATOM	338	CA ALA A	73	-18.796	38.175 103.008	1.00 50.87	С
MOTA	339	C ALA A	73	-18.268	36.767 102.760	1.00 47.48	c.
ATOM	340	O ALA A	73	-17.482	36.222 103.541	1.00 36.90	0
ATOM	341	CB ALA A	73 74	-20.237	38.098 103.464	1.00 61.96	C N
MOTA MOTA	342 343	N GLU A	74	-18.740 -18.331	36.181 101.666 34.851 101.257	1.00 48.41	C
ATOM	344	C GLU A	74	-16.810	34.785 101.268	1.00 44.48	č
ATOM	345	O GLU A	74	-16.215	33.957 101.959	1.00 35.80	0
ATOM	346	CB GLU A	74	-18.844	34.572 99.841	1.00 64.11	С
MOTA	347	CG GLU A	74	-19.454	33.198 99.656	1.00 88.13	C C
MOTA	348	CD GLU A	74	-18.490	32.075 99.998	1.00104.29	С
MOTA	349	OE1 GLU A	74	-17.493	31.893 99.263	1.00112.61	0
ATOM	350	OE2 GLU A	74	-18.733	31.376 101.008	1.00111.41	0
ATOM	351	N LEU A	75	-16.203	35.687 100.502 35.784 100.355	1.00 44.39	N
MOTA ATOM	352 353	CA LEU A	75 75	-14.754 -13.938	35.894 101.631	1.00 43.26 1.00 39.65	Ç
ATOM	354	O LEU A	75	-13.046	35.081 101.861	1.00 42.63	õ
ATOM	355	CB LEU A	75	-14.402	36.965 99.464	1.00 47.71	č
MOTA	356	CG LEU A	75	-14.719	36.813 97.981	1.00 56.06	Ċ
ATOM	357	CD1 LEU A	75	-16.201	36.526 97.782	1.00 66.62	000000
MOTA	358	CD2 LEU A	75	-14.308	38.085 97.255	1.00 64.54	С
MOTA	359	N MET A	76	-14.212	36.911 102.441	1.00 34.46	N
ATOM	360	CA MET A	76	-13.474	37.082 103.685	1.00 32.44	C C
MOTA	361	C MET A	76	-13.219	35.721 104.305	1.00 37.52	0
MOTA MOTA	362 363	O MET A	76 76	-12.145 -14.260	35.464 104.851 37.954 104.653	1.00 44.32 1.00 28.67	c
ATOM	364	CG MET A	76	-14.383	39.378 104.033	1.00 27.61	Č
ATOM	365	SD MET A	76	-15.332	40.382 105.305	1.00 43.61	S
ATOM	366	CE MET A	76	-14.098	40.677 106.578	1.00 48.42	С
ATOM	367	N VAL A	77	-14.220	34.853 104.196	1.00 41.86	N
MOTA	368	CA VAL A	77	-14.145	33.495 104.706	1.00 42.36	С
MOTA	369	C VAL A	77	-13.260	32.629 103.799	1.00 39.82	C
MOTA	370	O VAL A	77	-12.404	31.885 104.283	1.00 38.89	0
MOTA MOTA	371 372	CB VAL A	77 77	-15.545 -15.466	32.869 104.764 31.501 105.407	1.00 41.56 1.00 43.46	c c
ATOM	373	CG1 VAL A	77	-16.499	33.776 105.531	1.00 45.91	č
ATOM	374	N SER A		-13.476	32.750 102.489	1.00 36.14	N
ATOM	375	CA SER A		-12.734	32.010 101.476	1.00 42.45	С
MOTA	376	C SER A	78	-11.227	32.115 101.584	1.00 46.34	С
MOTA	377	O SER A	78	-10.578	31.218 102.117	1.00 54.34	0
MOTA	378	CB SER A		-13.152	32.462 100.077	1.00 47.24	C
ATOM	379	OG SER A		-14.527	32.205 99.847	1.00 62.25	0
MOTA	380	N GLU A		-10.660	33.196 101.059 33.385 101.098	1.00 48.13	N C
MOTA	381 382	CA GLU A		-9.207 -8.654	33.641 102.504	1.00 47.50	č
MOTA MOTA	383	C GLU A		-7.646	34.328 102.681	1.00 44.99	0
MOTA	384	CB GLU A		-8.795	34.554 100.201	1.00 51.38	Č
MOTA	385	CG GLU A		-9.060	34.326 98.722	1.00 58.71	c
MOTA	386	CD GLU A	79	-8.227	33.197 98.148	1.00 60.00	С
MOTA	387	OE1 GLU A		-7.038	33.090 98.515	1.00 66.35	0
MOTA	388	OE2 GLU A		-8.763	32.419 97.332	1.00 54.42 1.00 48.14	0 N
ATOM	389	N GLY A		-9.325 -8.893	33.071 103.498 33.188 104.876	1.00 48.14	C
MOTA MOTA	390 391	CA GLY A		-8.650	34.557 105.470	1.00 46.09	č
ATOM	392	O GLY A		-7.648	34.760 106.153	1.00 47.24	0
MOTA	393	N TRP A		-9.543	35.504 105.214	1.00 41.67	N
MOTA	394	CA TRP A	81	-9.399	36.836 105.796	1.00 34.07	C
MOTA	395	C TRP A		-9.847	36.737 107.248	1.00 33.67	c
MOTA	396	O TRP A	81	-9.191	37.240 108.160	1.00 32.32	0

N TO M	207	CD	TO D		10 270	37 047 10	NE 056	1 00 1	0 60	С
ATOM	397	CB	TRP .			37.847 10		1.00		
MOTA	398	CG	TRP .			38.170 10		1.00 2		C
MOTA	399		TRP .			37.669 10		1.00		C
MOTA	400		TRP .			39.035 10	03.416	1.00 2		С
MOTA	401		TRP .			38.170 10		1.00		N
MOTA	402		TRP .		-8.483	39.011 10	02.011	1.00		С
ATOM	403	CE3	TRP .	8 A	7.800	39.828 10	04.197	1.00 2	25.29	С
MOTA	404	CZ2	TRP .	A 8	7.480	39.750 10	01.370	1.00	38.96	С
ATOM	405	CZ3	TRP .	8 A	-6.805	40.561 10	33.562	1.00 2	27.92	С
MOTA	406	CH2	TRP .	8 A	-6.654	40.517 10		1.00	35.85	С
ATOM	407	N	LYS .			36.066 10		1.00 2		N
ATOM	408	CA	LYS			35.887 10		1.00 2		С
ATOM	409	C	LYS			35.315 10		1.00		C
ATOM	410	ŏ	LYS			35.859 1		1.00		Ō
ATOM	411	ČВ	LYS			34.947 10		1.00		č ·
MOTA	412	CG	LYS			34.802 1		1.00		č
MOTA	413	CD	LYS			34.104 10		1.00		č ·
			LYS			33.751 1		1.00		č
MOTA	414	CE				32.898 1		1.00		N
ATOM	415	NZ	LYS .			34.231 10		1.00		N
MOTA	416	N	ASP .							č
MOTA	417	CA	ASP .			33.550 10		1.00		č
MOTA	418	C	ASP .			34.490 1		1.00		ò
MOTA	419	0	ASP .			34.320 13		1.00		č
MOTA	420	CB	ASP .			32.452 10		1.00		Č
MOTA	421	CG	ASP .			31.372 10		1.00		
MOTA	422		ASP .			30.616 10		1.00		0
MOTA	423		ASP .			31.272 10		1.00		0
MOTA	424	N	ALA .			35.473 10		1.00 !		N
MOTA	425	CA	ALA			36.423 1		1.00		C
MOTA	426	C	ALA			37.464 1		1.00		C
MOTA	427	0	ALA	_		38.059 1		1.00		0
MOTA	428	CB	ALA			37.107 1		1.00		C
MOTA	429	N	GLY			37.690 1		1.00		N
MOTA	430	CA	GLY			38.666 1		1.00		C
MOTA	431	С	GLY			39.515 1		1.00		C
ATOM	432	0	GLY	a 8		39.805 1		1.00		0
MOTA	433	N	TYR	A 8		39.935 1		1.00		N
MOTA	434	CA	TYR					1.00		C
ATOM	435	С	TYR	a 8	-12.082			1.00		С
ATOM	436	0	TYR	А 8	-12.242			1.00		0
ATOM	437	CB	TYR	А 8	-10.655	41.047 1		1.00		С
MOTA	438	CG	TYR	A 8		41.665 1		1.00		С
MOTA	439	CD1	TYR	8 A	-9.104			1.00		С
MOTA	440	CD2	TYR	А 8				1.00		С
ATOM	441	CE1	TYR	A 8	-7.841	43.585 1	08.127	1.00	46.91	С
MOTA	442	CE2	TYR	A 8	-6.965	41.413 1	07.630	1.00	39.36	С
MOTA	443	CZ	TYR	A 8	-6.776	42.767 1	07.786	1.00	45.40	С
ATOM	444	ОН	TYR	A 8	-5.521	43.297 1	07.606	1.00	46.34	0
MOTA	445	N	GLU	A B	7 -12.964	40.526 1	11.011	1.00	39.34	N
ATOM	446	CA	GLU	A 8	7 -14.183	39.836 1	11.369	1.00	40.09	С
MOTA	447	С	GLU	A 8	7 -15.422	40.699 1	11.219	1.00	32.92	С
ATOM	448	0	GLU	A 8	7 -16.548	40.221 1	11.374	1.00	37.99	0
ATOM	449	CB	GLU	A 8	7 -14.041	39.339 1	12.799	1.00	52.92	С
ATOM	450	CG	GLU		7 -15.316	38.889 1	13.460	1.00	76.75	С
ATOM	451	CD	GLU		7 -15.068	38.461 1	14.891	1.00	93.47	С
ATOM	452		GLU		7 -14.373	39.206 1	15.617	1.001	00.50	0
ATOM	453		GLU					1.001	00.39	0
ATOM	454	N	TYR		-15.211	41.968 1	10.896	1.00	29.14	N
MOTA	455	CA	TYR	A 8		42.908 1	10.724	1.00	30.69	С
ATOM	456	С	TYR			43.390 1	09.285	1.00	32.71	C
MOTA	457	0	TYR			43.949 1		1.00	34.05	0
MOTA	458	СВ	TYR			44.119 1		1.00	20.03	С
ATOM	459	CG	TYR			43.888 1	13.081	1.00	20.03	С
ATOM	460		TYR			44.135 1	13.549	1.00	18.12	С
ATOM	461		TYR			43.443 1	13.985	1.00	19.14	С
MOTA	462		TYR			43.952 1	14.875	1.00	19.29	С
ATOM	463		TYR			43.254 1	15.321	1.00	26.80	С
ATOM	464	cz	TYR			43.513 1		1.00	26.99	С
ATOM	465	OH	TYR					1.00		0
ATOM	466	N	LEU			43.170 1	08.741	1.00		N
ATOM	467	CA	LEU					1.00		С
ATOM	468	Ċ	LEU			44.750 1		1.00	33.86	С
ATOM	469	ŏ	LEU			44.563 1		1.00		0
ATOM	470	ČВ	LEU					1.00		С
ATOM	471	CG	LEU			42.609 1	05.153	1.00		C
ATOM	472		LEU				04.383	1.00		С
ATOM	473		LEU			41.267 1	04.587	1.00		С
ATOM	474	N	CYS			45.942 1		1.00		N
ATOM	475	CA	CYS			47.092 1		1.00		C
MOTA	476	С	CYS		-19.899	47.915 1		1.00		C
ATOM	477	0	CYS		-19.133	48.143 1	05.222	1.00	40.56	0

MOTA		B CYS A	90	-18.823	47.994 108.362	1.00 32.78	¢
MOTA		G CYS A	90	-18.214	47.010 109.726	1.00 46.36	S
MOTA	480 N		91	-21.140	48.374 106.244	1.00 40.65	N
MOTA	481 C	A ILE A	91	-21.754	49.193 105.223	1.00 38.29	C
ATOM	482 C	ILE A	91	-21.589	50.643 105.610	1.00 39.61	С
ATOM	483 O	ILE A	91	-21.740	51.013 106.774	1.00 41.42	0
MOTA	484 C	B ILE A	91	-23.256	48.938 105.120	1.00 36.59	С
ATOM	485 C	G1 ILE A	91	-23.530	47.449 104.971	1.00 40.49	С
ATOM	486 C	G2 ILE A	91	-23.824	49.701 103.943	1.00 32.88	С
ATOM	487 C	D1 ILE A	91	-24.996	47.109 105.012	1.00 49.06	C
ATOM	488 N	ASP A	92	-21.284	51.461 104.616	1.00 38.83	N
MOTA		A ASP A	92	-21.113	52.879 104.831	1.00 41.57	С
MOTA	490 C		92	-22.311	53.587 104.201	1.00 41.21	С
ATOM	491 O		92	-23.258	52.934 103.768	1.00 49.28	0
ATOM		B ASP A	92	-19.796	53.343 104.207	1.00 42.41	С
ATOM		G ASP A	92	-19.438	54.766 104.596	1.00 43.83	С
ATOM		D1 ASP A	92	-19.865	55.691 103.865	1.00 51.06	0
ATOM		D2 ASP A	92	-18.750	54.950 105.637	1.00 19.32	0
MOTA	496 N		93	-22.266	54.912 104.154	1.00 38.07	N
ATOM		A ASP A	93	-23.345	55.718 103.600	1.00 37.38	С
ATOM	498 C		93	-23.908	55.187 102.283	1.00 33.12	С
MOTA	499 O		93	-23.263	54.396 101.577	1.00 23.80	0
ATOM		B ASP A	93	-22.847	57.142 103.381	1.00 40.75	. С
ATOM	501 C	G ASP A	93	-23.949	58.159 103.486	1.00 40.94	С
MOTA	502 C	D1 ASP A	93	-25.098	57.826 103.122	1.00 46.78	0
ATOM	503 C	D2 ASP A	93	-23.668	59.293 103.930	1.00 44.21	0
ATOM	504 N	CYS A	94	-25.128	55.613 101.967	1.00 31.07	N
ATOM		A CYS A	94	-25.773	55.230 100.714	1.00 33.68	С
ATOM	506 C		94	-26.370	53.830 100.663	1.00 29.32	С
ATOM	507 C		94	-26.602	53.281 99.595	1.00 33.63	Ō
ATOM		B CYS A	94	-24.777	55.426 99.564	1.00 32.58	С
MOTA		G CYS A	94	-24.368	57.192 99.335	1.00 56.68	S
ATOM	510 N		95	-26.644	53.261 101.821	1.00 24.27	N
ATOM		A TRP A	95	-27.224	51.929 101.891	1.00 30.02	C C
ATOM	512 C		95	-28.720	52.075 102.131	1.00 43.86	С
MOTA	513 C		95	-29.482	51.111 101.986	1.00 45.97	0
ATOM	514 C	B TRP A	95	-26.646	51.167 103.082	1.00 31.37	С
MOTA		G TRP A	95	-27.041	51.785 104.400	1.00 31.21	C
ATOM	516 C	D1 TRP A	95	-26.362	52.752 105.091	1.00 35.75	Ċ
ATOM	517 C	D2 TRP A	95	-28.234	51.520 105.152	1.00 30.42	С
ATOM	518 N	JE1 TRP A	95	-27.058	53.106 106.224	1.00 33.13	N
MOTA	519 C	E2 TRP A	95	-28.212	52.369 106.284	1.00 34.20	С
ATOM	520 C	E3 TRP A	95	-29.325	50.657 104.975	1.00 38.45	С
ATOM	521 C	ZZZ TRP A	95	-29.232	52.369 107.242	1.00 41.21	C
MOTA	522 C	Z3 TRP A	95	-30.344	50.661 105.934	1.00 46.80	Č
ATOM	523 C	CH2 TRP A	95	-30.288	51.515 107.047	1.00 47.81	С
MOTA	524 N	J MET A	96	-29.126	53.279 102.524	1.00 56.48	N
MOTA	525 C	A MET A	96	-30.514	53.544 102.853	1.00 60.38	Ç
ATOM	526 C	MET A	96	-31.398	54.078 101.742	1.00 59.84	С
ATOM	527 C	MET A	96	-30.953	54.774 100.828	1.00 53.40	0
MOTA	528 C	B MET A	96	-30.574	54.498 104.049	1.00 61.17	Ċ
ATOM	529 C	G MET A	96	-29.632	55.693 103.933	1.00 60.98	Ç
ATOM	530 S	D MET A	96	-29.696	56.754 105.387	1.00 57.31	ş
ATOM	531 C	E MET A	96	-29.014	55.691 106.626	1.00 49.16	С
ATOM	532 N		97	-32.671	53.725 101.839	1.00 59.61	N
MOTA		CA ALA A	97	-33.664	54.198 100.903	1.00 57.58	ç
ATOM	534 C		97	-33.879	55.656 101.316	1.00 58.35	C
MOTA	535 C		97	-33.478	56.067 102.405	1.00 63.58	0
ATOM		B ALA A	97	-34.935	53.409 101.058	1.00 59.55	Ç
MOTA	537 N		98	-34.501	56.457 100.446	1.00 57.40	N
MOTA		A PRO A	98	-34.811	57.880 100.607	1.00 57.23	c
MOTA	539 C		98	-35.465	58.376 101.881	1.00 61.14	c
MOTA	540 C		98	-35.261	59.528 102.252	1.00 62.28	0
MOTA		B PRO A	98	-35.651	58.174 99.389	1.00 60.63	C C
MOTA		G PRO A	98	-34.989	57.331 98.364	1.00 68.69	c
MOTA		D PRO A	98	-34.859	56.015 99.092	1.00 59.58	
MOTA	544 N		99	-36.275	57.551 102.535	1.00 68.09 1.00 73.61	N C
ATOM		CA GLN A	99	-36.894	57.990 103.784	1.00 73.61	c
ATOM	546 0		99	-37.551	56.923 104.630	1.00 75.40	Ö
ATOM	547 0		99 99	-37.772 -37.910	55.790 104.201	1.00 80.81	Ċ
MOTA		CB GLN A	99	-37.910	59.118 103.550 58.723 102.815	1.00 80.34	Ċ
MOTA			99	-39.168	58.557 101.330	1.00 89.00	ċ
ATOM ATOM		D GLN A E1 GLN A	99	-38.264	57.625 100.890	1.00 92.41	ŏ
MOTA		JEI GLIN A JE2 GLN A	99	-39.498	59.473 100.545	1.00 89.50	N
MOTA	553 N			-37.851	57.345 105.851	1.00 75.98	N
MOTA		ARG A		-38.464	56.537 106.885	1.00 80.55	č
MOTA	555 0			-39.716	55.842 106.399	1.00 82.57	č
ATOM	556			-40.319	56.259 105.414	1.00 80.59	ŏ
ATOM		CB ARG A		-38.823	57.435 108.069	1.00 80.70	č
ATOM		G ARG A		-37.709	58.391 108.501	1.00 75.07	č

		~~			100	36 -35				_
MOTA	559	CD	arg			-36.739	57.726	109.462	1.00 64.10	С
MOTA	560	NE	ARG	Α	100	-35.661	58.621	109.876	1.00 52.24	N
ATOM	561	CZ	ARG	Α	100	-34.704	58.281	110.733	1.00 47.35	С
MOTA	562	NH1	ARG	Α	100	-34.693		111.271	1.00 40.85	N
MOTA	563		ARG			-33.751		111.039	1.00 47.99	N
	564									
MOTA		N	ASP			-40.101		107.103	1.00 86.12	N
ATOM	565	CA	ASP			-41.307	54.038	106.760	1.00 92.31	С
ATOM	566	С	ASP	Α	101	-42.496	54.603	107.536	1.00 98.60	С
ATOM	567	0	ASP	Α	101	-42.369	55.594	108.268	1.00 92.38	0
ATOM	568	СВ	ASP	А	101	-41.144		107.023	1.00 88.34	Ċ
	569	CG	ASP							č
ATOM						-40.924		108.502	1.00 78.93	Č
ATOM	570		ASP			-41.624	52.699		1.00 78.59	0
ATOM	571	OD2	ASP	Α	101	-40.062	51.292	108.791	1.00 69.58	0
ATOM	572	N	SER	Α	102	-43.657	53.987	107.347	1.00106.35	N
ATOM	573	CA	SER	Α	102	-44.866		108.030	1.00106.95	С
ATOM	574	C	SER		102	-44.581		109.520	1.00105.57	č
	575									
ATOM		0	SER			-45.012		110.180	1.00103.49	0
ATOM	576	CB	SER			-45.991		107.772	1.00106.67	С
MOTA	577	OG	SER	Α	102	-45.534	52.081	107.928	1.00 97.92	0
ATOM	578	N	GLU	Α	103	-43.834	53.550	110.029	1.00104.74	N
MOTA	579	CA	GLU	Α	103	-43.456		111.437	1.00105.44	С
ATOM	580	C	GLU			-42.482		111.787	1.00 99.30	č
		ŏ								
ATOM	581		GLU			-42.400		112.936	1.00 97.60	0
ATOM	582	CB	GLU		103	-42.808		111.733	1.00120.87	Ç
ATOM	583	CG	GLU	Α	103	-42.725	51.763	113.207	1.00138.34	С
ATOM	584	CD	GLU	Α	103	-44.085	51.428	113.796	1.00149.87	С
ATOM	585		GLU	Α	103	-44.777		113.228	1.00156.42	0
ATOM	586		GLU			-44.461		114.830	1.00153.81	ŏ
			GLY						1.00 93.42	N
ATOM	587	N				-41.730		110.799		
ATOM	588	CA	GLY			-40.790		111.053	1.00 86.33	Ç
ATOM	58 9	С	GLY	Α	104	-39.355	55.715	111.299	1.00 80.52	С
ATOM	590	0	GLY	Α	104	-38.530	56.511	111.741	1.00 76.38	0
ATOM	591	N	ARG	Α	105	-39.055	54.451	111.023	1.00 74.97	N
ATOM	592	CA	ARG			-37.701		111.194	1.00 66.50	Ĉ
						-37.060		109.821		č
ATOM	593	C	ARG						1.00 62.55	
ATOM	594	0	ARG			-37.726		108.827	1.00 61.70	0
ATOM	595	CB	ARG	Α	105	-37.728	52.500	111.665	1.00 67.28	С
ATOM	596	CG	ARG	Α	105	-38.680	52.241	112.790	1.00 71.50	C
ATOM	597	CD	ARG			-38.708		113.114	1.00 81.08	C
MOTA	598	NE	ARG			-39.129		114.489	1.00101.63	N
										ċ
ATOM	599	CZ	ARG			-39.140		115.086	1.00112.71	
MOTA	600	NH1				-38.755		114.427	1.00117.25	N
MOTA	601	NH2	ARG	Α	105	-39.529	49.259	116.350	1.00120.85	N
ATOM	602	N	LEU	Α	106	-35.774	53.694	109.743	1.00 57.99	N
MOTA	603	CA	LEU			-35.119	53.714	108.449	1.00 53.74	С
ATOM	604	c	LEU			-35.525		107.615	1.00 52.72	č
								107.966	1.00 59.39	ŏ
ATOM	605	0	LEU		106	-36.427				
ATOM	606	CB	LEU		106	-33.618		108.642	1.00 49.89	C
ATOM	607	CG	LEU	Α	106	-33.326		109.573	1.00 53.87	С
ATOM	608	CD1	LEU	Α	106	-32.012	54.646	110.288	1.00 56.85	С
ATOM	609	CD2	LEU	Α	106	-33.332	56.182	108.782	1.00 65.81	С
ATOM	610	N	GLN		107	-34.838		106.500	1.00 49.03	N
ATOM	611	CA	GLN		107	-35.108		105.601	1.00 50.68	Ċ
						-34.066		104.529	1.00 47.10	č
ATOM	612	C	GLN		107	-34.000				
MOTA	613	0	GLN		107	-33.730		104.059	1.00 46.93	0
ATOM	614	CB	GLN		107	-36.501		104.990	1.00 64.70	С
ATOM	615	CG	GLN	Α	107	-36.833	52.801	104.492	1.00 75.71	С
ATOM	616	CD	GLN	Α	107	-38.271	52.926	104.010	1.00 77.30	С
ATOM	617		GLN		107	-39.179		104.619	1.00 78.88	0
ATOM	618					-38.483		102.920	1.00 74.52	N
			GLN			-33.530		104.171	1.00 44.21	N
ATOM	619	N	ALA							
ATOM	620	CA	ALA			-32.523		103.134	1.00 45.01	C
ATOM	621	С	ALA			-33.214		101.806	1.00 46.03	С
ATOM	622	0	ALA	Α	108	-34.401	50.040	101.675	1.00 45.34	0
MOTA	623	CB	ALA	Α	108	-31.853	48.748	103.158	1.00 50.26	С
ATOM	624	N	ASP			-32.468	50.792	100.824	1.00 50.12	N
ATOM	625	CA	ASP			-33.011	51.006	99.495	1.00 58.74	č
ATOM	626		ASP			-33.751	49.727	99.096	1.00 60.18	č
		C							1.00 60.18	
ATOM	627	0	ASP			-33.189	48.636	99.117		0
ATOM	628	CB	ASP			-31.876	51.288	98.524	1.00 65.46	C
MOTA	629	CG	ASP			-32.368	51.750	97.184	1.00 69.48	c
ATOM	630	OD1	ASP	Α	109	-32.987	52.833	97.132	1.00 77.79	0
ATOM	631		ASP			-32.134	51.036	96.186	1.00 64.36	0
ATOM	632	N	PRO			-35.029	49.850	98.725	1.00 63.63	N
ATOM	633	CA	PRO			-35.869	48.718	98.328	1.00 68.57	ċ
						-35.279	47.860	97.227	1.00 68.18	č
	634	č	PRO							č
MOTA	635	0	PRO			-35.295	46.633	97.303	1.00 69.60	0
ATOM	636	CB	PRO			-37.157	49.390	97.871	1.00 72.56	C
ATOM	637	CG	PRO			-37.174	50.668	98.646	1.00 71.02	c
ATOM	638	CD	PRO	Α	110	-35.750	51.117	98.532	1.00 68.06	c
MOTA	639	N	GLN	Α	111	-34.761	48.523	96.201	1.00 69.52	N

MOTA	640	CA	GLN A	111	-34.185	47.846	95.047	1.00	69.50	С
MOTA	641	С	GLN A	111	-32.822	47.199	95.308	1.00	65.01	С
ATOM	642	ŏ	GLN A		-32.589	46.057	94.915		69.57	ŏ
MOTA	643	CB	GLN A		-34.075	48.831	93.877		77.55	C
MOTA	644	CG	GLN A	111	-35.379	49.542	93.519	1.00	91.86	С
MOTA	645	CD	GLN A	111	-35.797	50.560	94.562	1.00	95.66	С
ATOM	646		GLN A		-35.040	51.469	94.889		97.70	0
							95.083		90.78	
MOTA	647		GLN A		-37.009	50.415				N
ATOM	648	N	ARG A	112	-31.933	47.925	95.979	1.00	57.71	N
ATOM	649	CA	ARG A	112	-30.598	47.416	96.278	1.00	49.91	С
ATOM	650	Ċ	ARG A		-30.535	46.547	97.551		46.94	С
MOTA	651	0	ARG A		-29.542	45.863	97.803		39.87	0
MOTA	652	CB	ARG A	112	-29.614	48.597	96.367	1.00	48.63	С
MOTA	653	CG	ARG A	112	-29.482	49.367	95.056	1.00	49.72	С
ATOM	654	CD	ARG A		-28.531	50.554	95.113	1.00	46.10	С
			ARG A			51.668				
ATOM	655	NE			-29.063		95.887		52.81	N
ATOM	656	CZ	ARG A	112	-28.722	51.919	97.144	1.00	68.43	С
ATOM	657	NH1	ARG A	112	-27.848	51.127	97.747	1.00	79.08	N
ATOM	658		ARG A		-29.252	52.948	97.801		75.10	N
ATOM	659	N	PHE A		-31.605	46.555	98.339		50.25	N
ATOM	660	CA	PHE A	113	-31.642	45.774	99.572	1.00	50.71	С
ATOM	661	С	PHE A	113	-33.074	45.326	99.850	1.00	52.92	С
ATOM	662	Ó	PHE A		-33.640		100.900		57.25	0
		_							54.24	
ATOM	663	CB	PHE A		-31.136		100.737			C
MOTA	664	CG	PHE A	113	-29.684	47.023	100.625	1.00	58.84	С
ATOM	665	CD1	PHE A	113	-28.674	46.090	100.823	1.00	59.23	С
ATOM	666		PHE A		-29.326		100.319		66.37	С
										č
MOTA	667		PHE A		-27.327		100.722		55.58	C
ATOM	668	CE2	PHE A	113	-27.981	48.710	100.214	1.00	63.98	C
ATOM	669	CZ	PHE A	113	-26.983	47.770	100.415	1.00	57.08	С
ATOM	670	N	PRO A		-33.669	44.582	98.906	1.00	50.78	N
					-35.027	44.021	98.887		48.50	Ċ
ATOM	671	CA	PRO A							-
ATOM	672	С	PRO A		-35.381		100.057		47.73	С
ATOM	673	0	PRO A	114	-36.490	43.204	100.600	1.00	46.16	0
MOTA	674	CB	PRO A	114	-35.054	43.253	97.581	1.00	50.90	С
ATOM	675	ĊĠ	PRO A		-33.655	42.742	97.506		45.72	č
			-							~
ATOM	676	CD	PRO A		-32.867	43.985	97.826		47.08	С
ATOM	677	N	HIS A	115	-34.445	42.265	100.431	1.00	44.63	N
ATOM	678	CA	HIS A	115	-34.681	41.365	101.545	1.00	53.14	С
ATOM	679	c	HIS A		-34.580		102.892		58.55	Č
										~
ATOM	680	0	HIS A		-35.210		103.854		65.19	0
ATOM	681	CB	HIS A	115	-33.699	40.204	101.489	1.00	47.76	С
ATOM	682	CG	HIS A	115	-33.849	39.356	100.268	1.00	46.31	С
ATOM	683		HIS A		-35.061	38.833	99.874		57.77	N
ATOM	684		HIS A		-32.941	38.931	99.359		42.56	C
ATOM	685	CE1	HIS A	115	-34.894	38.123	98.773	1.00	58.00	С
ATOM	686	NE2	HIS A	115	-33.617	38.166	98.440	1.00	53.03	N
ATOM	687	N	GLY A		-33.794		102.954		55.93	N
										Ċ
ATOM	688	CA	GLY A		-33.649		104.193		49.77	
ATOM	689	C	GLY A	116	-32.440		105.028		42.46	C
ATOM	690	0	GLY A	116	-31.990	42.392	105.052	1.00	41.59	0
ATOM	691	N	ILE A	117	-31.916	44.529	105.734	1.00	38.38	N
ATOM	692	CA	ILE A		-30.746		106.580		30.95	Ċ
										~
ATOM	693	С	ILE A		-30.837		107.412		35.65	C
MOTA	694	0	ILE A	117	-30.069	42.125	107.194	1.00	40.26	0
MOTA	695	CB	ILE A	117	-30.531	45.455	107.565	1.00	26.18	С
ATOM	696		ILE A		-30.420		106.810		19.83	С
ATOM	697		ILE A		-29.275		108.344		16.45	Č
				_						
ATOM	698		ILE A		-29.218		105.923	1.00	3.31	C
ATOM	699	N	ARG A	118	-31.761	43.038	108.375	1.00	39.17	N
ATOM	700	CA	ARG A		-31.912	41.872	109.239	1.00	49.23	С
ATOM	701	c.	ARG A		-31.394		108.531		53.14	č
MOTA	702	0	ARG A		-30.312		108.835		56.73	0
MOTA	703	CB	ARG A		-33.369		109.601		56.41	С
ATOM	704	CG	ARG A	118	-33.605	40.231	110.201	1.00	62.55	С
ATOM	705	CD	ARG A		-35.066		110.216		64.78	Ċ
										N
MOTA	706	NE	ARG A		-35.876		110.985		78.48	
ATOM	707	CZ	ARG A		-36.212		110.575		83.25	C
ATOM	708	NH1	ARG A	118	-35.816	42.420	109.389	1.00	85.88	N
ATOM	709	NH2			-36.932		111.363		85.50	N
ATOM	710	N	GLN A		-32.169		107.568		51.32	N
MOTA	711	CA	GLN A		-31.766		106.843		49.87	C
MOTA	712	С	GLN A		-30.331		106.368		46.58	С
MOTA	713	0	GLN A	119	-29.608	38.035	106.468	1.00	53.92	0
MOTA	714	ČВ	GLN A		-32.705		105.681		53.02	Č
									62.39	
MOTA	715	CG	GLN A		-33.884		106.104			C
MOTA	716	CD	GLN A	119	-34.912		105.014		65.61	С
ATOM	717	OE1	GLN A	119	-34.610	37.145	103.961	1.00	72.73	0
MOTA	718		GLN A		-36.132		105.259		65.96	N
MOTA	719	N					105.877		38.64	N
			LEU A		-29.904					
		4.4	LEU A	120	-28.531	40.306	105.432	1.00	27.87	С
MOTA	720	CA	DLU A							•

MOTA	721	C	LEU	Α	120		. 623	39.860	106.580	1.00	23.13	С
ATOM	722	0	LEU	A	120	-26	.772	38.972	106.436	1.00	19.96	0
ATOM	723	CB	LEU	Α	120	-28	. 235	41.764	105.072	1.00	24.63	С
ATOM	724	CG	LEU	Α	120	-26	.786	42.073	104.710		17.89	č
ATOM	725		LEU			-26	. 377	41.287	103.496	1.00	3.31	Č
ATOM	726		LEU			-26			104.450		28.71	č
ATOM	727	N	ALA			-27			107.729		20.79	Ň
	728	CA	ALA			-27			108.943			
ATOM						-27			109.224		30.72	C
ATOM	729	Č	ALA								38.03	C
ATOM	730	0	ALA			-25.			109.460		42.89	0
ATOM	731	СВ	ALA			-27.			110.134		31.00	C
ATOM	732	N	ASN			-28			109.190		40.73	N
ATOM	733	CA	ASN			-28			109.466	1.00	46.05	С
ATOM	734	С	ASN			-27			108.567	1.00	45.38	С
ATOM	735	0	ASN			-26.			109.003	1.00	47.50	0
MOTA	736	CB	ASN	Α	122	-29.	623	36.127	109.319	1.00	56.34	С
ATOM	737	CG	ASN	Α	122	-30.	617	36.961	110.080	1.00	64.60	C
ATOM	738	OD1	ASN	Α	122	-30.	. 363	37.361	111.216	1.00	61.74	0
MOTA	739	ND2	ASN	Α	122	-31.	762	37.231	109.465	1.00	79.71	N
MOTA	740	N	TYR			-27.			107.312		40.88	N
ATOM	741	CA	TYR			-26.			106.413		45.83	Ċ
ATOM	742	Ċ	TYR			-24.			106.936		41.18	č
ATOM	743	ō	TYR			-24.			107.163		40.91	ŏ
ATOM	744	СВ	TYR			-26			104.975		54.03	č
ATOM	745	CG	TYR			-25.			104.037		62.59	č
	746											Ċ
ATOM			TYR			-25.			103.722		75.25	c
ATOM	747		TYR			-24.			103.535		55.30	c
ATOM	748	CEI	TYR			-24.			102.943		76.30	Č
ATOM	749		TYR			-23.			102.762		58.81	Ċ
MOTA	750	CZ	TYR			-23.			102.468		71.09	Ċ
ATOM	751	ОН	TYR			~22.			101.722		67.72	0
ATOM	752	N	VAL			-24.			107.131		36.55	N
MOTA	753	CA	VAL	Α	124	-23.	. 293	37.555	107.648	1.00	30.58	С
MOTA	754	С	VAL	Α	124	-22.			108.906	1.00	26.95	С
ATOM	755	0	VAL	Α	124	-21.	779	36.317	109.063	1.00	21.59	0
ATOM	756	CB	VAL	Α	124	-23.	350	39.040	108.005	1.00	35.31	С
ATOM	757	CG1	VAL			-21.		39.563	108.313	1.00	38.27	Ċ
MOTA	758	CG2	VAL	Α	124	-23.		39.806	106.867	1.00	32.66	С
ATOM	759	N	HIS			-23.	888	36.571	109.801		25.84	N
ATOM	760	CA	HIS			-23.			111.001		27.43	Ċ
ATOM	761	Ċ	HIS			-23.			110.638		25.94	č
ATOM	762	ŏ	HIS			-22.			111.128		20.70	ŏ
ATOM	763	СВ	HIS			-24.			112.012		42.27	č
	764											
ATOM	765	CG	HIS			-24.			112.466		51.98	C
			HIS			-23.			113.049		54.13	N
	766		HIS			-26.			112.437		51.03	C
ATOM	767		HIS			-24.			113.358		49.04	C
ATOM	768		HIS			-25.			112.997		47.54	N
	769	N	SER			-24.			109.768		23.94	N
	770	CA	SER			-24.			109.332		26.69	С
	771	Ç	SER			-22.			108.886		28.55	С
ATOM	772	0	SER			-22.			109.131		30.63	0
MOTA	773	CB	SER	Α	126	-25.	382	32.193	108.258	1.00	20.10	С
MOTA	774	OG	SER	Α	126	-25.			107.874		25.00	0
ATOM	775	N	LYS	Α	127	-22.	298	33.135	108.230	1.00	31.85	N
ATOM	776	CA	LYS	Α	127	-20.		32.984	107.755	1.00	36.73	С
ATOM	777	С	LYS	Α	127	-19.	890	33.326	108.835	1.00	36.08	С
ATOM	778	0	LYS	Α	127	-18.	692	33.452	108.541	1.00	39.60	0
MOTA	779	CB	LYS	Α	127	-20.		33.852	106.514	1.00	33.46	С
	780	CG	LYS			-21.			105.342		47.96	С
	781	CD	LYS			-20.			104.228		46.23	С
	782	CE	LYS			-20.			104.698		50.82	, C
	783	NZ	LYS			-19.			103.587		57.29	N
	784	N	GLY			-20.			110.070		34.48	N
	785	CA	GLY			-19.			111.194		34.06	С
	786	C	GLY			-18.			111.378		36.68	Ċ
	787	ō	GLY			-18.			112.319		35.44	ŏ
	788	N	LEU			-19.			110.503		36.41	Ň
	789	CA	LEU			-18.			110.591		33.42	Ċ
	790	c	LEU			-19.			111.318		37.65	č
	791	ō	LEU			-21.			111.673		43.74	ŏ
	792	СB	LEU			-18			109.190		28.00	č
	793	CG	LEU			-17.			108.435		37.07	č
	794		LEU			-17.			106.945		36.47	č
	795		LEU			-16.			100.943		31.18	Č
	796	N	LYS			-19.			111.534		38.98	N
	797	CA	LYS			-20.			112.200		38.49	Č
	798	C	LYS			-20.			111.232		37.28	Č
	799	ŏ	LYS			-19.			110.530		33.90	ŏ
	800	СВ				-19.			113.489			č
	801	CG	LYS			-19.			114.370		39.52	Č
	JU1		LYS	^	130	-17.	202		-14.370	1.00	50.59	C

MOTA	802	CD		A 130	-19.089	40.247	115.858	1.00 60.9	
MOTA	803	CE	LYS .	A 130	-18.735	39.035	116.736	1.00 65.0	2 C
ATOM	804	NZ	LYS .	A 130	-19.726		116.647	1.00 72.5	8 N
ATOM	805	N		A 131	-21.790		111.184	1.00 38.7	
ATOM	806	CA		A 131	-22.164		110.289	1.00 34.9	
MOTA	807	С		A 131	-22.144	44.712	110.935	1.00 33.7	
MOTA	808	0	LEU .	A 131	-22.399	44.868	112.136	1.00 41.7	
MOTA	809	CB	LEU .	A 131	-23.559	43.087	109.715	1.00 37.9	4 C
	810	CG		A 131	-24.239			1.00 37.7	
MOTA							109.135		
MOTA	811		LEU .		-23.559		107.839	1.00 44.1	1 C
ATOM	812	CD2	LEU .	A 131	-25.718	44.042	108.905	1.00 49.6	3 C
ATOM	813	N	GLY .	A 132	-21.861	45.718	110.116	1.00 23.7	9 N
ATOM	814	CA		A 132	-21.821		110.599	1.00 25.4	
				A 132	-22.558		109.644	1.00 24.7	
ATOM	815	C							
ATOM	816	0		A 132	-22.493		108.419	1.00 24.3	
MOTA	817	N	ILE .	A 133	-23.252	48.989	110.198	1.00 26.8	
ATOM	818	CA	ILE .	A 133	-24.004	49.914	109.373	1.00 27.5	8 C
ATOM	819	C	ILE .	A 133	-23.593		109.633	1.00 22.9	
	820	ŏ		A 133	-23.066		110.695	1.00 19.2	
ATOM									
MOTA	821	СВ		A 133	-25.498		109.632	1.00 27.2	3 C
MOTA	822	CG1	ILE .	A 133	-26.298	50.513	108.584	1.00 33.1	
ATOM	823	CG2	ILE .	A 133	-25.817	50.200	111.044	1.00 35.1	6 C
ATOM	824		ILE .		-26.139		107.205	1.00 36.2	3 C
ATOM	825	N		A 134	-23.850		108.641	1.00 28.1	
							108.697		
MOTA	826	CA		A 134	-23.514			1.00 32.0	
ATOM	827	С		A 134	-24.745		109.061	1.00 31.5	8 C
ATOM	828	0	TYR .	A 134	-25.849	54.081	108.676	1.00 31.0	
MOTA	829	CB	TYR .	A 134	-22.971	54.035	107.326	1.00 42.1	8 C
ATOM	830	CG		A 134	-22.758		107.114	1.00 42.7	q c
							106.963	1.00 51.1	ć
MOTA	831		TYR .		-21.473				
ATOM	832	CD2	TYR .		-23.843		107.026	1.00 49.2	
MOTA	833	CE1	TYR .	A 134	-21.281	57.405	106.725	1.00 55.3	7 C
ATOM	834	CE2	TYR .	A 134	-23.663	57.735	106.791	1.00 53.5	7 C
MOTA	835	CZ		A 134	-22.383		106.640	1.00 53.1	8 C
	836	ОН		A 134	-22.224		106.398	1.00 60.1	
ATOM									
MOTA	837	N		A 135	-24.552		109.798	1.00 31.6	
ATOM	838	CA	ALA .	A 135	- 25 . 657	56.405	110.200	1.00 34.8	5 C
ATOM	839	С	ALA .	A 135	-25.128	57.806	110.372	1.00 35.2	5 C
ATOM	840	0		A 135	-23.920	58.004	110.371	1.00 35.8	0 0
ATOM	841	ČВ		A 135	-26.265		111.507	1.00 30.4	
MOTA	842	N		A 136	-26.017		110.524	1.00 29.2	
MOTA	843	CA	ASP .	A 136	-25.558		110.717	1.00 28.0	2 C
MOTA	844	С	ASP .	A 136	-26.319	60.894	111.805	1.00 25.3	
MOTA	845	0	ASP .	A 136	-27.544	60.892	111.848	1.00 28.9	7 0
ATOM	846	ČВ		A 136	-25.629		109.416	1.00 30.5	
					-24.689		109.435	1.00 31.2	Ž C
ATOM	847	CG		A 136					1
ATOM	848			A 136	-24.857		110.301	1.00 3.3	
ATOM	849	OD2	ASP .	A 136	-23.771		108.588	1.00 35.2	
ATOM	850	N	VAL .	A 137	-25.559	61.542	112.670	1.00 24.0	6 N
ATOM	851	CA	VAL.	A 137	-26.111	62.284	113.782	1.00 29.1	7 C
ATOM	852	Ċ		A 137	-27.011		113.405	1.00 27.7	
							114.108	1.00 18.7	
ATOM	853	0		A 137	-27.982				2 0
MOTA	854	CB	VAL .	A 137	-24.993		114.683	1.00 29.1	ي و
ATOM	855	CG1	VAL .	A 137	-24.305	64.015	113.946	1.00 37.0	3 C
MOTA	856	CG2	VAL .	A 137	-25.569	63.343	115.990	1.00 28.0	8 C
ATOM	857	N	GLY .	A 138	-26.678	64.120	112.315	1.00 33.1	
ATOM	858	CA		A 138	-27.453		111.911	1.00 46.0	
							111.159	1.00 51.0	
ATOM	859	C		A 138	-28.739				
MOTA	860	0	GLY .	A 138	-29.370	63.984	111.297	1.00 56.7	_
MOTA	861	N	ASN .	A 139	-29.112		110.348	1.00 53.5	
MOTA	862	CA	ASN .	A 139	-30.332	65:951	109.563	1.00 50.3	4 C
MOTA	863	Ċ		A 139	-30.175	65.110	108.258	1.00 41.5	0 C
MOTA	864	ō		A 139	-31.166		107.598	1.00 34.9	
								1.00 62.9	
MOTA	865	CB		A 139	-30.839		109.281		
MOTA	866	CG		A 139	-31.173		110.578	1.00 71.5	
ATOM	867	QD1	ASN .	A 139	-31.352		111.627	1.00 71.8	
MOTA	868			A 139	-31.259	69.515	110.510	1.00 81.7	5 N
MOTA	869	N		A 140	-28.945	64.726	107.907	1.00 37.3	5 N
ATOM	870	CA		A 140	-28.668		106.717	1.00 35.8	
				A 140			106.831	1.00 38.2	
MOTA	871	Č			-27.304				1 ^
MOTA	872	0		A 140	-26: 441		107.586	1.00 44.3	
ATOM	873	CB		A 140	-28.640		105.433	1.00 29.8	S C
ATOM	874	CG	LYS .	A 140	-29.974		104.795	1.00 40.4	9 C
ATOM	875	CD		A 140	-29.785		103.584	1.00 62.5	2 C
ATOM	876	CE		A 140	-31.122		103.054	1.00 70.2	
	877	NZ			-30.972		102.015	1.00 70.6	
ATOM				A 140			106.085		
MOTA	878	N		A 141	-27.115				, C
MOTA	879	CA		A 141	-25.838		106.076	1.00 35.5	<u>0</u> C
MOTA	880	С		A 141	-25.039		105.118	1.00 36.9	
MOTA	881	0		A 141	-25.639		104.405	1.00 42.5	
ATOM	882	CB		A 141	-25.975	60.033	105.472	1.00 32.9	3 C
				_					

MOTA	883	OG1	THR	Δ	141	-26.291	60 140	104.084	1.00	29.61	0
ATOM	884		THR			-27.092		106.139		39.81	č
	885	N	CYS			-23.714				38.49	N
MOTA			CYS					105.077		44.01	
	886	CA				-22.977		104.136		44.89	c
ATOM	887	C	CYS			-23.473		102.724			Č
MOTA	888	0	CYS			-23.156		101.806		50.35	0
ATOM	889	СВ	CYS			-21.459		104.205		51.38	C
ATOM	890	SG	CYS			-20.666		105.784		72.02	S
ATOM	891	N	ALA			-24.270		102.566		45.64	N
ATOM	892	CA	ALA			-24.804		101.263		52.01	С
ATOM	893	С	ALA			-26.059		100.901		59.39	С
ATOM	894	0	ALA			-26.345	62.316	99.726		63.73	0
ATOM	895	CB	ALA			-25.106		101.220		54.75	C
ATOM	896	N	GLY			-26.806		101.905		63.40	N
MOTA	897	CA	GLY			-28.025		101.642		68.16	С
ATOM	898	С	GLY			-29.212		102.121		67.45	C
ATOM	899	0	GLY	A	144	-30.330	62.996	102.269		73.47	0
ATOM	900	N	PHE			-28.963		102.373		61.79	N
ATOM	901	CA	PHE	Α	145	-30.022	60.351	102.843	1.00	57.87	С
ATOM	902	С	PHE	Α	145	-30.378	60.634	104.292	1.00	54.82	С
ATOM	903	0	PHE	Α	145	-29.678	61.390	104.967	1.00	52.34	0
ATOM	904	CB	PHE	A	145	-29.584	58.898	102.698	1.00	56.96	С
ATOM	905	CG	PHE	Α	145	-29.472	58.447	101.282	1.00	58.46	С
ATOM	906	CD1	PHE	Α	145	-30.591	58.397	100.479	1.00	63.62	С
MOTA	907	CD2	PHE	Α	145	-28.246	58.096	100.744	1.00	56.83	С
ATOM	908	CE1	PHE	Α	145	-30.500	58.028	99.150	1.00	71.78	С
ATOM	909	CE2	PHE	Α	145	-28.141	57.727	99.423	1.00	62.21	С
MOTA	910	CZ	PHE	A	145	-29.271	57.684	98.618	1.00	69.70	С
MOTA	911	N	PRO	Α	146	-31.477	60.038	104.777	1.00	56.74	N
ATOM	912	CA	PRO	A	146	-31.988	60.176	106.139	1.00	60.73	С
MOTA	913	С	PRO	A	146	-30.920	60.463	107.166	1.00	59.16	С
ATOM	914	0	PRO	Α	146	-29.834	59.916	107.090	1.00	67.99	0
ATOM	915	CB	PRO			-32.670	58.843	106.361	1.00	65.25	С
ATOM	916	CG	PRO			-33.358	58.661	105.042	1.00	70.30	С
ATOM	917	CD	PRO			-32.298	59.078	104.015	1.00	60.08	С
ATOM	918	N	GLY			-31.254	61.312	108.130		54.04	N
ATOM	919	CA	GLY			-30.312		109.168		49.65	С
ATOM	920	C	GLY			-30.484		110.331		46.61	С
ATOM	921	ō	GLY			-30.271		110.187		50.36	0
ATOM	922	N	SER			-30.897		111.471		43.80	N
ATOM	923	CA	SER			-31.109		112.677		48.24	Ċ
ATOM	924	Ċ	SER			-31.480		113.800		54.21	Ċ
ATOM	925	ō	SER			-31.791		114.918		55.54	ō
MOTA	926	ČВ	SER			-29.846		113.062		42.87	Ċ
ATOM	927	ŌĞ	SER			-29.742		112.350		45.45	ŏ
ATOM	928	N	PHE			-31.434		113.484		60.50	N
MOTA	929	CA	PHE			-31.753		114.438		61.79	Ċ
ATOM	930	Ċ	PHE			-33.112		115.045		64.22	č
ATOM	931	ŏ	PHE			-34.107		114.329		64.91	Õ
ATOM	932	ČВ	PHE			-31.753		113.741		65.43	č
ATOM	933	ĊĠ	PHE			-31.915		114.675		67.92	č
ATOM	934		PHE			-31.151		115.829		65.58	Ċ
ATOM	935		PHE			-32.825		114.405		76.80	č
ATOM	936		PHE			-31.280		116.705		75.12	č
ATOM	937		PHE			-32.968		115.274		83.75	č
ATOM	938	CZ	PHE			-32.193		116.432		83.27	č
ATOM	939	N	GLY			-33.157		116.365		67.83	Ñ
ATOM	940	CA	GLY			-34.424		117.020		74.79	Ċ
ATOM	941	c	GLY			-35.020		116.581		76.82	c
ATOM	942	ŏ	GLY			-36.199		116.244		87.25	ŏ
ATOM	943	N	TYR			-34.190		116.562		71.76	N
ATOM	944	CA	TYR			-34.624		116.160		66.00	Ċ
ATOM	945	c	TYR			-33.688		116.817		61.26	č
ATOM	946	ŏ	TYR			-33.960		116.851		56.60	ō
ATOM	947	СВ	TYR			-34.529		114.639		73.54	č
ATOM	948	CG	TYR			-35.575		113.820		76.28	č
ATOM	949		TYR			-36.916		113.809		82.28	č
ATOM	950		TYR			-35.210		113.001		79.60	č
ATOM	951		TYR			-37.857		113.007		84.58	č
ATOM	952		TYR			-36.142		112.209		86.91	č
ATOM	953	CZ	TYR			-37.458		112.210		85.18	č
ATOM	954	OH	TYR			-38.361		111.399		84.45	ŏ
ATOM	955	N	TYR			-32.577		117.332		57.27	N
ATOM	956	CÁ	TYR			-31.556		117.980		56.78	c c
ATOM	957	Č	TYR			-32.129		118.610		56.79	č
ATOM	958	ō	TYR			-31.900		118.122		59.65	ŏ
ATOM	959	ČВ	TYR			-30.833		119.038		57.11	С
ATOM	960	CG	TYR			-30.262		118.493		51.41	č
ATOM	961		TYR			-29.449		117.356		45.75	Ċ
ATOM	962		TYR			-30.543		119.106		52.15	Č
ATOM	963		TYR			-28.934		116.844		40.47	Ċ

MOTA	964	CE2	TYR A	A 152	-30.030	62.680 118.602	1.00 50.45	С
		-	TYR A		-29.228		1.00 41.43	
MOTA	965	CZ				62.661 117.472		C
MOTA	966	ОН	TYR A		-28.723	63.839 116.972	1.00 33.76	0
MOTA	967	N	ASP A	A 153	-32.879	57.068 119.692	1.00 53.39	N
ATOM	968	CA	ASP A	A 153	-33.479	55.931 120.369	1.00 59.36	С
ATOM	969	Ċ	ASP A		-34.119	54.968 119.363	1.00 61.05	č
MOTA	970	0	ASP A		-33.724	53.806 119.279	1.00 69.33	0
MOTA	971	CB	ASP A		-34.519	56.409 121.383	1.00 61.10	С
ATOM	972	CG	ASP A	A 153	-33.905	57.192 122.522	1.00 66.61	С
MOTA	973	OD1	ASP A	153	-32.967	56.666 123.159	1.00 74.47	0
ATOM	974		ASP A		-34.368	58.324 122.785	1.00 67.84	ŏ
ATOM	975	N	ILE A		-35.089	55.446 118.590	1.00 58.54	N
MOTA	976	CA	ILE A	A 154	-35.744	54.590 117.603	1.00 56.48	С
ATOM	977	C	ILE A	A 154	-34.714	53.813 116.799	1.00 53.07	С
ATOM	978	0	ILE A	154	-34.649	52.584 116.868	1.00 55.38	0
ATOM	979	ČВ	ILE A		-36.582	55.402 116.607	1.00 60.62	č
MOTA	980		ILE A		-37.745	56.075 117.331	1.00 60.11	Č
MOTA	981	CG2	ILE A	A 154	-37.103	54.491 115.510	1.00 58.52	С
ATOM	982	CD1	ILE A	A 154	-38.627	56.910 116.424	1.00 68.47	С
MOTA	983	N	ASP A	155	-33.915	54.548 116.034	1.00 49.17	N
ATOM	984	CA	ASP A		-32.881	53.949 115.207	1.00 48.75	c
MOTA	985	C	ASP A		-32.097	52.895 115.975	1.00 46.33	C
MOTA	986	0	ASP A		-31.971	51.757 115.531	1.00 47.70	0
MOTA	987	CB	ASP A	155	-31.941	55.038 114.687	1.00 56.70	С
ATOM	988	CG	ASP A	155	-32.637	55.999 113.730	1.00 65.61	С
ATOM	989		ASP A		-31.990	56.962 113.255	1.00 66.95	ō
ATOM	990		ASP A		-33.837	55.786 113.447	1.00 76.23	ŏ
MOTA	991	N	ALA A		-31.575	53.271 117.133	1.00 43.12	N
MOTA	992	CA	ALA A		-30.819	52.323 117.934	1.00 51.16	С
ATOM	993	С	ALA A	156	-31.570	50.994 118.019	1.00 57.39	С
MOTA	994	0	ALA A	156	-31.122	49.981 117.488	1.00 54.91	0
ATOM	995	ČВ	ALA A		-30.580	52.890 119.330	1.00 54.88	Č
MOTA	996	N	GLN A		-32.723	51.004 118.676	1.00 62.27	N
MOTA	997	CA	GLN A		-33.515	49.791 118.815	1.00 62.11	С
MOTA	998	С	GLN A	1 157	-33.610	49.115 117.454	1.00 58.35	С
MOTA	999	0	GLN A	157	-33.424	47.901 117.336	1.00 55.24	0
ATOM	1000	СB	GLN A		-34.918	50.122 119.333	1.00 66.46	Č
ATOM	1001	CG	GLN A					
					-35.418	49.129 120.344	1.00 68.51	C
MOTA	1002	CD	GLN A		-34.542	49.106 121.575	1.00 73.20	С
ATOM	1003		GLN A		-34.440	50.103 122.291	1.00 72.76	0
MOTA	1004	NE2	GLN A	157	-33.893	47.971 121.825	1.00 73.79	N
MOTA	1005	N	THR A		-33.895	49.907 116.425	1.00 55.78	N
ATOM	1006	CA	THR A		-34.001	49.375 115.076	1.00 57.61	c
MOTA	1007	Ċ	THR A		-32.802	48.459 114.822	1.00 59.20	Č
MOTA	1008	0	THR A	158	-32.946	47.236 114.805	1.00 59.18	0
MOTA	1009	CB	THR A	158	-34.012	50.508 114.017	1.00 59.39	C
ATOM	1010	OG1	THR A	158	-35.156	51.348 114.216	1.00 58.60	0
MOTA	1011		THR A		-34.061	49.927 112.619	1.00 59.01	Ċ
ATOM	1012		PHE A		-31.621	49.056 114.651	1.00 58.19	Ň
		N						
ATOM	1013	CA	PHE A		-30.387	48.299 114.398	1.00 52.96	Č
ATOM	1014	С	PHE A	1 159	-30.257	47.139 115.368	1.00 51.83	С
MOTA	1015	0	PHE A	159	-30.010	45.998 114.966	1.00 52.13	0
MOTA	1016	CB	PHE A	159	-29.148	49.174 114.588	1.00 39.41	С
ATOM	1017	CG	PHE A		-29.164	50.447 113.803	1.00 33.46	Ċ
			PHE A		-29.153	50.425 112.414		č
MOTA	1018	-					1.00 40.11	
MOTA	1019		PHE A		-29.158	51.677 114.456	1.00 27.14	Ç
ATOM	1020			159	-29.131	51.608 111.687	1.00 39.56	С
MOTA	1021	CE2	PHE A	159	-29.136	52.861 113.744	1.00 26.61	С
ATOM	1022	CZ	PHE A		-29.122	52.829 112.353	1.00 29.93	Ċ
ATOM	1023	N	ALA A		-30.396	47.457 116.651	1.00 46.49	N
					-30.293	46.467 117.705	1.00 51.93	c
MOTA	1024	CA	ALA A					
ATOM	1025	c	ALA A		-31.140	45.256 117.363	1.00 53.81	C
ATOM	1026	0	ALA A		-30.736	44.121 117.612	1.00 57.70	0
MOTA	1027	CB	ALA A	160	-30.743	47.071 119.021	1.00 56.28	С
MOTA	1028	N	ASP A		-32.312	45.502 116.779	1.00 52.03	N
ATOM	1029	CA	ASP A		-33.213	44.420 116.399	1.00 48.71	Ċ
								č
ATOM	1030	Č	ASP A		-32.813	43.799 115.066	1.00 46.99	
MOTA	1031	0	ASP A		-32.960	42.603 114.869	1.00 47.02	0
MOTA	1032	CB	ASP A		-34.654	44.918 116.321	1.00 54.43	С
ATOM	1033	CG	ASP A	161	-35.135	45.513 117.628	1.00 64.53	С
ATOM	1034		ASP A		-34.756	44.987 118.695	1.00 66.37	0
ATOM	1035		ASP A		-35.905	46.498 117.589	1.00 73.72	ŏ
			TRP A		-32.305		1.00 42.60	N
MOTA	1036	N				44.615 114.151		
ATOM	1037	CA	TRP A		-31.864	44.130 112.848	1.00 47.02	C
ATOM	1038	C	TRP A		-30.728	43.135 112.995	1.00 52.84	c
ATOM	1039	0	TRP A	162	-30.453	42.347 112.079	1.00 58.41	0
ATOM	1040	CB	TRP A		-31.391	45.296 111.996	1.00 45.23	С
ATOM	1041	ĊĞ	TRP A		-32.495	46.058 111.387	1.00 52.02	c c
ATOM	1042		TRP A			45.819 111.517	1.00 57.35	č
ATOM	1042				-33.829		1.00 55.31	c
		L.132	TRP A	162	-32.365	47.164 110.506	1 00 33.31	
ATOM	1044		TRP A		-34.542	46.710 110.761	1.00 58.06	N

								_
MOTA	1045	CE2	TRP A	162	-33.666	47.549 110.127	1.00 54.33	С
ATOM	1046	CE3	TRP A	162	-31.273	47.868 109.992	1.00 57.11	С
MOTA	1047	CZ2			-33.907	48.610 109.258	1.00 54.11	C
MOTA	1048		TRP A		-31.509	48.923 109.129	1.00 54.12	С
MOTA	1049	CH2	TRP A	162	-32.819	49.284 108.769	1.00 56.13	С
MOTA	1050	N	GLY A	163	-30.071	43.190 114.153	1.00 50.47	N
MOTA	1051	CA	GLY A		-28.960			Ċ
						42.301 114.435	1.00 48.75	
MOTA	1052	С	GLY A		-27.611	42.895 114.074	1.00 48.13	С
MOTA	1053	0	GLY A	163	-26.724	42.194 113.586	1.00 49.04	0
ATOM	1054	N	VAL A	164	-27.452	44.188 114.321	1.00 46.12	N
MOTA	1055	CA	VAL A		-26.203	44.862 114.015	1.00 39.85	Ç
MOTA	1056	С	VAL A	164	-25.140	44.616 115.068	1.00 41.90	С
ATOM	1057	0	VAL A	164	-25.442	44.341 116.231	1.00 48.62	0
MOTA	1058	CB	VAL A		-26.404	46.364 113.896	1.00 32.22	С
			VAL A		-25.117			č
ATOM	1059					47.018 113.440	1.00 37.25	
MOTA	1060	CG2	VAL A	164	-27.540	46.650 112.934	1.00 23.64	С
ATOM	1061	N	ASP A	165	-23.888	44.721 114.650	1.00 40.76	N
ATOM	1062	CA	ASP A		-22.779	44.513 115.559	1.00 46.54	С
							1.00 47.34	
ATOM	1063	Ċ	ASP A		-21.925	45.765 115.675		Ċ
ATOM	1064	0	ASP A	165	-21.208	45.941 116.660	1.00 50.94	0
ATOM	1065	CB	ASP A	165	-21.900	43.362 115.074	1.00 43.91	C
ATOM	1066	CG	ASP A	165	-22.657	42.066 114.949	1.00 45.91	С
ATOM	1067		ASP A		-23.265	41.617 115.956	1.00 49.23	ŏ
ATOM	1068		ASP A		-22.632	41.503 113.833	1.00 41.28	0
ATOM	1069	N	LEU A		-21.995	46.638 114.678	1.00 41.70	N
ATOM	1070	CA	LEU A	166	-21.184	47.849 114.708	1.00 34.79	С
ATOM	1071	C	LEU A		-21.817	49.022 113.966	1.00 29.04	č
MOTA	1072	0	LEU A		-22.388	48.849 112.883	1.00 18.18	0
ATOM	1073	CB	LEU A	166	-19.803	47.541 114.120	1.00 34.97	С
ATOM	1074	CG	LEU A	166	-18.748	48.640 113.932	1.00 28.60	С
ATOM	1075		LEU A		-17.429	47.992 113.523	1.00 32.34	č
ATOM	1076		LEU A		-19.198	49.642 112.875	1.00 34.11	C
ATOM	1077	N	LEU A	167	-21.685	50.217 114.545	1.00 29.90	N
ATOM	1078	CA	LEU A	167	-22.242	51.431 113.950	1.00 29.38	С
ATOM	1079	Ċ	LEU A		-21.230	52.536 113.652	1.00 30.39	Ċ
			LEU A					
MOTA	1080	0			-20.507	52.980 114.543	1.00 34.52	Ō
ATOM	1081	CB	LEU A		-23.313	52.022 114.865	1.00 29.92	. C
ATOM	1082	CG	LEU A	167	-23.849	53.353 114.333	1.00 26.86	C
ATOM	1083	CD1	LEU A	167	-24.617	53.072 113.056	1.00 23.49	С
ATOM	1084		LEU A		-24.741	54.042 115.356	1.00 24.77	č
ATOM	1085	N	LYS A		-21.185	52.985 112.404	1.00 31.63	N
ATOM	1086	CA	LYS A	168	-20.294	54.083 112.055	1.00 33.02	С
ATOM	1087	С	LYS A	168	-21.154	55.328 112.122	1.00 34.61	C
ATOM	1088	0	LYS A		-21.947	55.583 111.216	1.00 37.40	Ö
ATOM	1089	CB	LYS A		-19.733	53.936 110.631	1.00 36.20	Ċ
ATOM	1090	CG	LYS A	168	-18.885	55.153 110.176	1.00 36.63	С
ATOM	1091	CD	LYS A	168	-18.140	54.939 108.840	1.00 32.72	С
ATOM	1092	CE	LYS A		-17.230	56.127 108.494	1.00 17.31	С
ATOM	1093	NZ	LYS A		-16.338	55.854 107.338	1.00 20.64	Ñ
MOTA	1094	N	PHE A		-21.019	56.097 113.193	1.00 34.82	N
ATOM	1095	ÇA	PHE A	169	-21.830	57.292 113.320	1.00 43.12	С
MOTA	1096	С	PHE A	169	-21.143	58.538 112.769	1.00 44.70	C
ATOM	1097	Ō	PHE A		-20.330	59.169 113.444	1.00 46.72	ō
ATOM	1098	ČВ	PHE A		-22.227	57.498 114.780		č
							1.00 53.78	
ATOM	1099	CG	PHE A	169	-23.554	58.160 114.946	1.00 66.20	С
MOTA	1100	CD1	PHE A	169	-24.658	57.695 114.241	1.00 71.04	С
ATOM	1101	CD2	PHE A	169	-23.704	59.248 115.793	1.00 69.28	С
ATOM	1102	CEL	PHE A	169	-25.893	58.301 114.373	1.00 73.13	С
ATOM	1103		PHE A		-24.938	59.864 115.936	1.00 74.53	Ċ
ATOM	1104	CZ	PHE A		-26.037	59.389 115.223	1.00 75.63	C
ATOM	1105	N	ASP A		-21.493	58.886 111.534	1.00 43.70	N
ATOM	1106	CA	ASP A	170	-20.942	60.050 110.834	1.00 43.57	С
ATOM	1107	С	ASP A		-21.627	61.342 111.313	1.00 47.05	Ċ
ATOM	1108	ŏ	ASP A		-22.725	61.298 111.863	1.00 58.65	ŏ
ATOM	1109	CB	ASP A		-21.158	59.870 109.327	1.00 42.08	C
MOTA	1110	CG	ASP A	170	-20.438	60.894 108.510	1.00 47.03	С
ATOM	1111	OD1	ASP A	170	-19.948	61.874 109.086	1.00 39.35	0
ATOM	1112		ASP A		-20.365	60.724 107.282	1.00 60.53	Ó
ATOM	1113	N	GLY A		-20.991	62.490 111.096	1.00 40.64	Ň
ATOM	1114	CA	GLY A		-21.585	63.740 111.533	1.00 40.10	C
ATOM	1115	С	GLY A		-21.687	64.883 110.535	1.00 41.45	С
ATOM	1116	0	GLY A	171	-21.069	65.936 110.721	1.00 38.61	0
ATOM	1117	N	CYS A		-22.461	64.686 109.474	1.00 45.62	N
MOTA	1118	CA	CYS A		-22.662	65.740 108.485	1.00 57.26	ċ
MOTA	1119	Ç	CYS A		-24.014	66.376 108.765	1.00 64.15	c
ATOM	1120	0	CYS A		-24.971	65.671 109.085	1.00 68.98	0
ATOM	1121	CB	CYS A	172	-22.685	65.170 107.064	1.00 63.70	С
ATOM	1122	SG	CYS A		-21.108	65.199 106.143	1.00 78.74	Š
ATOM	1123	N	TYR A		-24.092	67.698 108.666	1.00 65.75	Ñ
ATOM	1124	CA	TYR A		-25.359	68.398 108.865	1.00 65.04	c
MOTA	1125	С	TYR A	173	-25.910	68.529 110.289	1.00 70.36	С

MOTO	1126	^	TYR	Δ	173	-26.614	67 643	110.768	1 00	68.61	C
MOTA	1126	0									
MOTA	1127	CB	TYR	Α	1/3	-26.444		108.004		50.88	C
MOTA	1128	CG	TYR	Α	173	-26.119	67.665	106.530	1.00	40.15	C
MOTA	1129		TYR			-25.907		105.783		44.16	Č
MOTA	1130		TYR			-26.058		105.874		37.10	C
MOTA	1131	CE1	TYR	Α	173	-25.645	68.764	104.416	1.00	35.52	C
MOTA	1132	CF2	TYR	Α	173	-25.800	66.368	104.507	1.00	32.18	Ċ
											_
ATOM	1133	CZ	TYR			-25.593		103.778		30.22	C
ATOM	1134	ОН	TYR	Α	173	-25.336	67.471	102.418	1.00	19.17	O
MOTA	1135	N	CYS	Α	174	-25.617	69.647	110.950	1.00	78.94	N
	1136	CA	CYS			-26.119		112.300		85.57	Ċ
MOTA		_									
MOTA	1137	С	CYS	Α	1/4	-25.742		112.742		94.32	C
MOTA	1138	0	CYS	Α	174	-24.630	71.778	112.500	1.001	103.79	C
MOTA	1139	CB	CYS			-25.584	68 879	113.296	1 00	78.87	C
						-23.805		113.299		61.30	
MOTA	1140	SG	CYS								S
ATOM	1141	N	ASP	Α	175	-26.684	71.995	113.390	1.00	97.67	N
MOTA	1142	CA	ASP	Α	175	-26.490	73.365	113.850	1.001	103.74	C
ATOM	1143	C	ASP			-25.154		114.555	1 001	103.67	Č
											,
ATOM	1144	0	ASP			-24.156		113.914		101.24	C
ATOM	1145	CB	ASP	Α	175	-27.653	73.783	114.769	1.00	117.72	C
MOTA	1146	CG	ASP	Α	175	-28.943	74.107	114.002	1.001	125.68	C
ATOM	1147		ASP			-28.928		113.134		131.47	ō
MOTA	1148	OD2	ASP			-29.982		114.280		135.80	O
ATOM	1149	N	SER	Α	176	-25.135	73.481	115.875	1.001	105.67	N
MOTA	1150	CA	SER			-23.914		116.637		109.70	C
ATOM	1151	c	SER			-23.466		117.357		108.65	č
MOTA	1152	0	SER			-24.222		117.444		105.77	0
MOTA	1153	CB	SER	Α	176	-24.140	74.827	117.660	1.001	116.59	C
MOTA	1154	OG	SER			-25.073		118.649		127.13	O
MOTA	1155	N	LEU			-22.236		117.870		109.10	N
MOTA	1156	CA	LEU	Α	177	-21.706	71.315	118.594	1.001	113.27	C
ATOM	1157	C	LEU	Α	177	-22.719	70.852	119.626	1.001	118.00	C
MOTA	1158	Ó	LEU	Δ	177	-22.741		120.002		19.05	Ö
ATOM	1159	CB	LEU			-20.395		119.289		108.56	C
MOTA	1160	CG	LEU	Α	177	-19.213	72.035	118.388	1.001	108.26	C
ATOM	1161	CD1	LEU	Α	177	-18.937	73.593	118.503	1.001	110.81	C
MOTA	1162		LEU			-17.984		118.755		13.74	C
	1163							120.096			
ATOM		N	GLU			-23.551				121.90	N
MOTA	1164	CA	GLU	Α	178	-24.593	71.419	121.053	1.001	126.02	C
MOTA	1165	С	GLU	Α	178	-25.284	70.201	120.449	1.001	120.33	C
MOTA	1166	0	GLU	A	178	-25.169		120.966		21.32	o
ATOM	1167	ČВ	GLU								č
						-25.601		121.215		138.76	<u> </u>
ATOM	1168	CG	GLU	Α	178	-25.076	73.783	121.982	1.001	152.42	C
MOTA	1169	CD	GLU	Α	178	-24.864	73.486	123.456	1.001	157.35	C
MOTA	1170		GLU			-25.854		124.136		57.22	Ō
ATOM	1171		GLU			-23.713		123.935		160.51	0
ATOM	1172	N	ASN	А	179	-25.968	70.409	119.328	1.001	110.14	N
MOTA	1173	CA	ASN	Α	179	-26.658	69.318	118.657	1.001	100.76	C
MOTA	1174	С	ASN	Α	179	-25.709		118.385		93.18	C
ATOM	1175	ŏ	ASN			-26.093		118.519		92.47	ō
MOTA	1176	СВ	ASN			-27.270		117.352		104.39	C
ATOM	1177	CG	ASN	Α	179	-28.245	70.946	117.569	1.001	102.16	C
MOTA	1178	OD1	ASN	Α	179	-28.886	71.040	118.620	1.00	90.92	0
MOTA	1179		ASN			-28.381		116.567		06.80	N
ATOM	1180	N	LEU			-24.469		118.020		81.89	N
MOTA	1181	CA	LEU	Α	180	-23.463		117.730	1.00	72.86	C
MOTA	1182	С	LEU	Α	180	-23.087	66.647	118.976	1.00	69.25	C
MOTA	1183	ō	LEU			-23.545		119.161		71.22	ō
								117.137			č
ATOM	1184	СВ	LEU	_		-22.204				70.11	_
ATOM	1185	CG	LEU	Α	180	-21.033		116.768	1.00	67.68	C
MOTA	1186	CD1	LEU	Α	180	-21.462	66.225	115.671	1.00	76.29	C
MOTA	1187		LEU			-19.854		116.309		65.37	Ċ
MOTA	1188	N	ALA			-22.245		119.820		64.43	N
MOTA	1189	CA	ALA			-21.802		121.044		66.82	C
MOTA	1190	С	ALA	Α	181	-22.922	65.761	121.672	1.00	65.66	C
MOTA	1191	Ó	ALA			-22.753		121.912		68.03	0
MOTA	1192	СВ	ALA			-21.291		122.034			č
										69.43	
MOTA	1193	N	ASP			-24.062		121.926		62.37	N
MOTA	1194	CA	ASP	Α	182	-25.206	65.715	122.524	1.00	65.99	C
MOTA	1195	С	ASP			-25.622		121.719		65.00	C
MOTA	1196	ŏ	ASP			-25.816		122.274		59.17	ō
MOTA	1197	CB	ASP			-26.406		122.656		73.88	C
MOTA	1198	CG	ASP			-26.334	67.525	123.893	1.00	80.02	C
MOTA	1199	OD1	ASP			-26.076		124.988		92.51	0
MOTA	1200		ASP			-26.547		123.779		75.90	ō
ATOM	1201	N	GLY			-25.767		120.409		66.05	N
MOTA	1202	CA	GLY			-26.156		119.543		60.45	C
MOTA	1203	С	GLY			-25.245		119.683	1.00	54.15	С
MOTA	1204	0	GLY	Α	183	-25.724		119.881	1.00	58.09	0
MOTA	1205	N	TYR			-23.933		119.576		45.07	N
ATOM	1206							119.711			Ċ
	1400	CA	TYR	^	104	-22.985	01.403	417./11	1.00	37.39	C

						-		
ATOM	1207	С	TYR	A 184	-23.210	60.856 121.067	1.00 34.36	С
							1.00 32.57	
ATOM	1208	0		A 184	-23.520	59.670 121.156		0
MOTA	1209	СВ	TYR A	A 184	-21.548	61.986 119.596	1.00 31.49	С
MOTA	1210	CG	TYR A	A 184	-21.003	61.897 118.190	1.00 28.45	C
MOTA	1211		TYR A		-20.770	60.661 117.584	1.00 34.59	С
ATOM	1212	CD2		A 184	-20.758	63.045 117.444	1.00 23.65	č
								Č
MOTA	1213	CE1			-20.306	60.574 116.266	1.00 34.51	Ç
ATOM	1214	CE2	TYR /	A 184	-20.296	62.966 116.124	1.00 26.31	С
MOTA	1215	CZ	TYR A	A 184	-20.074	61.729 115.548	1.00 29.11	С
MOTA	1216	ОH		A 184	-19.620	61.660 114.259	1.00 26.35	ō
MOTA	1217	N		A 185	-23.074	61.662 122.120	1.00 39.05	N
MOTA	1218	CA	LYS /	A 185	-23.277	61.193 123.495	1.00 48.75	С
MOTA	1219	С	LYS	A 185	-24.603	60.447 123.636	1.00 50.42	С
MOTA	1220	ō		A 185	-24.643	59.297 124.074	1.00 50.83	Ō
							1.00 58.43	
ATOM	1221	CB		A 185	-23.276	62.371 124.488		Č
MOTA	1222	CG	LYS /	A 185	-21.929	63.073 124.702	1.00 73.82	,C
MOTA	1223	CD	LYS A	A 185	-21.890	63.906 126.010	1.00 82.36	С
MOTA	1224	CE	LYS A	A 185	-22.888	65.063 126.016	1.00 93.18	С
MOTA	1225	NZ		A 185	-22.795	65.897 127.254	1.00 96.90	N
MOTA	1226	N		A 186	-25.686	61.121 123.263	1.00 52.77	N
MOTA	1227	CA	HIS A	A 186	-27.025	60.558 123.347	1.00 49.62	С
ATOM	1228	С	HIS A	A 186	-27.078	59.169 122.737	1.00 41.58	С
ATOM	1229	ō		A 186	-27.262	58.180 123.441	1.00 37.23	Ō
								č
MOTA	1230	CB		A 186	-28.017	61.472 122.634	1.00 54.01	C
MOTA	1231	CG		A 186	-29.447	61.124 122.894	1.00 57.63	С
MOTA	1232	ND1	HIS A	A 186	-30.497	61.799 122.305	1.00 59.91	N
MOTA	1233		HIS A		-30.007	60.178 123.684	1.00 60.61	С
	1234						1.00 65.11	č
MOTA			HIS A		-31.638	61.283 122.720		
MOTA	1235	NE2	HIS A	A 186	-31.369	60.296 123.558	1.00 64.41	- N
MOTA	1236	N	MET A	A 187	-26.919	59.104 121.421	1.00 36.42	N
MOTA	1237	CA		A 187	-26.930	57.837 120.702	1.00 37.19	С
MOTA	1238	Ċ		A 187	-26.125	56.778 121.468	1.00 39.71	č
								Č
MOTA	1239	0		A 187	-26.606	55.662 121.703	1.00 43.37	Ō
MOTA	1240	CB	MET A	A 187	-26.347	58.050 119.299	1.00 27.48	С
MOTA	1241	CG	MET A	A 187	-26.191	56.785 118.456	1.00 34.76	С
MOTA	1242	SD	MET A	A 187	-27.734	55.889 118.163	1.00 36.92	S
	1243	CE		A 187	-28.259		1.00 45.04	č
MOTA						56.613 116.581		
MOTA	1244	N	SER A	A 188	-24.909	57.149 121.866	1.00 41.71	N
ATOM	1245	CA	SER A	A 188	-24.017	56.263 122.600	1.00 37.27	С
MOTA	1246	С	SER A	A 188	-24.764	55.527 123.699	1.00 31.50	С
MOTA	1247	ŏ		A 188	-24.648	54.312 123.837	1.00 29.93	ō
		_						, i
MOTA	1248	CB		A 188	-22.873	57.066 123.205	1.00 39.51	. С
MOTA	1249	OG	SER A	A 188	-21.937	56.205 123.826	1.00 38.33	0
MOTA	1250	N	LEU A	A 189	-25.537	56.274 124.474	1.00 30.93	N
ATOM	1251	CA		A 189	-26.326	55.706 125.562	1.00 38.86	Ċ
								č
MOTA	1252	C		A 189	-27.498	54.864 125.034	1.00 37.08	
MOTA	1253	0	LEU A	A 189	-27.819	53.795 125.578	1.00 34.46	0
MOTA	1254	CB	LEU A	A 189	-26.871	56.840 126.434	1.00 51.38	С
ATOM	1255	CG		A 189	-25.869	57.868 126.964	1.00 55.89	Ċ
ATOM	1256		LEU A		-26.630	59.095 127.449	1.00 62.91	č
								Č
ATOM	1257		LEU A		-25.018	57.255 128.078	1.00 48.77	C
MOTA	1258	N	ALA A	A 190	-28.136	55.367 123.979	1.00 34.71	N
ATOM	1259	CA	ALA A	A 190	-29.266	54.689 123.364	1.00 36.52	С
ATOM	1260	С		A 190	-28.897	53.247 123.064	1.00 41.07	Ċ
MOTA	1261	ŏ		A 190	-29.653	52.325 123.367	1.00 45.62	ō
								ŭ
ATOM	1262	CB		A 190	-29.662	55.397 122.092	1.00 32.84	C
MOTA	1263	N	LEU A	A 191	-27.724	53.060 122.473	1.00 41.81	N
ATOM	1264	CA	LEU A	A 191	-27.240	51.733 122.133	1.00 43.27	С
ATOM	1265	Ċ		A 191	-27.056	50.828 123.359	1.00 45.92	С
MOTA	1266	ŏ		A 191	-27.756	49.827 123.502	1.00 46.02	ŏ
ATOM	1267	CB		A 191	-25.931	51.865 121.354	1.00 38.79	c
ATOM	1268	CG		A 191	-26.052	52.702 120.071	1.00 38.54	С
ATOM	1269	CD1	LEU A	A 191	-24.669	52.980 119.495	1.00 40.68	С
MOTA	1270		LEU A		-26.916	51.970 119.045	1.00 41.30	С
ATOM	1271	N		A 192	-26.125	51.160 124.245	1.00 50.32	N
						50.314 125.412		Č
MOTA	1272	CA		A 192	-25.933		1.00 51.94	<u> </u>
MOTA	1273	Ç		A 192	-27.311	49.916 125.898	1.00 51.27	C
MOTA	1274	0		A 192	-27.566	48.751 126.184	1.00 53.27	0
ATOM	1275	CB	ASN A	A 192	-25.190	51.056 126.523	1.00 51.78	С
ATOM	1276	CG		A 192	-24.865	50.153 127.715	1.00 51.63	č
MOTA	1277		ASN A		-25.766	49.594 128.339	1.00 64.23	ŏ
MOTA	1278		ASN A		-23.574	50.016 128.021	1.00 45.03	N
MOTA	1279	N	ARG A	A 193	-28.209	50.893 125.945	1.00 55.36	N
MOTA	1280	CA	ARG A	A 193	-29.565	50.653 126.400	1.00 62.45	С
ATOM	1281	C		A 193	-30.216	49.485 125.669	1.00 55.61	Ċ
ATOM	1282	õ		A 193	-30.807	48.608 126.295	1.00 59.33	ŏ
								ŏ
ATOM	1283	CB		A 193	-30.403	51.910 126.207	1.00 73.86	c
MOTA	1284	CG		A 193	-31.760	51.866 126.876	1.00 95.58	С
MOTA	1285	CD	ARG A	A 193	-32.437	53.194 126.676	1.00110.48	Ċ
MOTA	1286	NE		A 193	-31.459	54.266 126.821	1.00120.92	N
		CZ		A 193	-31.697	55.547 126.561	1.00125.94	Ċ
MOTA	1287							

MOTA	1288	NH1	ARG A	193	-32.892	55.935	126.141	1.00130.65	N
MOTA	1289	NH2	ARG A	193	-30.732	56.444	126.713	1.00126.19	N
MOTA	1290	N	THR A		-30.100		124.345	1.00 43.02	N
MOTA	1291	CA	THR A		-30.702		123.546	1.00 36.14	С
MOTA	1292	С	THR A	194	-30.298	47.013	124.034	1.00 32.48	С
MOTA	1293	0	THR A	194	-31.037	46.044	123.835	1.00 29.14	0
ATOM	1294	ĊВ	THR A		-30.297		122.069	1.00 35.70	Č
MOTA	1295	OG1			-28.926		121.938	1.00 35.73	0
MOTA	1296	CG2	THR A	194	-30.475	49.900	121.535	1.00 39.30	С
MOTA	1297	N	GLY A	195	-29.121	46.918	124.652	1.00 30.85	N
MOTA	1298	CA	GLY A		-28.651		125.154	1.00 34.30	C
MOTA	1299	C	GLY A		-27.734		124.193	1.00 36.49	Ċ
MOTA	1300	0	GLY A	195	-26.890		124.600	1.00 36.19	0
ATOM	1301	N	ARG A	196	-27.905	45.163	122.906	1.00 40.82	N
MOTA	1302	CA	ARG A	196	-27.087	44.538	121.876	1.00 46.67	С
ATOM	1303		ARG A		-25.670		122.013	1.00 48.09	č
		C							
MOTA	1304	0	ARG A		-25.489		122.195	1.00 54.78	0
ATOM	1305	CB	ARG A	196	-27.673	44.870	120.490	1.00 54.84	С
ATOM	1306	CG	ARG A	196	-26.968	44.253	119.286	1.00 63.61	С
ATOM	1307	CD	ARG A		-27.506		118.919	1.00 72.08	Ċ
ATOM	1308	NE	ARG A		-26.709		117.848	1.00 77.41	Ŋ
ATOM	1309	CZ	ARG A	196	-26.723	41.002	117.514	1.00 85.11	С
MOTA	1310	NH1	ARG A	196	-27.499	40.145	118.159	1.00 84.72	N
ATOM	1311		ARG A		-25.936	40 569	116.544	1.00 93.60	N
	1312		SER A		-24.667		121.955	1.00 45.00	N
ATOM		N							
MOTA	1313	CA	SER A		-23.276		122.050	1.00 44.47	Ç
MOTA	1314	С	SER A	197	-22.887	45.261	120.692	1.00 50.27	. с
MOTA	1315	0	SER A	197	-22.621	44.519	119.740	1.00 55.75	0
ATOM	1316	ČВ	SER A		-22.367		122.371	1.00 41.44	č
MOTA	1317	OG	SER A		-22.822		123.524	1.00 44.41	0
MOTA	1318	N	ILE A	198	-22.846	46.591	120.603	1.00 49.87	N
MOTA	1319	CA	ILE A	198	-22.519	47.278	119.343	1.00 46.63	С
ATOM	1320	C	ILE A		-21.248		119.359	1.00 41.34	С
			ILE A				120.042	1.00 44.43	
ATOM	1321	0_			-21.197				0
MOTA	1322	CB	ILE A		-23.663		118.911	1.00 47.20	С
MOTA	1323	CG1	ILE A	198	-25.025	47.552	119.043	1.00 45.40	С
MOTA	1324	CG2	ILE A	198	-23.441	48.687	117.481	1.00 47.83	C
ATOM	1325		ILE A		-26.198		118.835	1.00 31.46	Č
MOTA	1326	N	VAL A		-20.227		118.602	1.00 35.54	N
MOTA	1327	CA	VAL A	199	-19.019	48.561	118.560	1.00 33.21	С
MOTA	1328	С	VAL A	199	-19.430	49.899	117.960	1.00 25.97	С
ATOM	1329	ō	VAL A		-19.899		116.823	1.00 21.07	Ö
									č
MOTA	1330	CB	VAL A		-17.919		117.673	1.00 37.47	_
MOTA	1331	CG1	VAL A	199	-16.794	48.968	117.472	1.00 34.52	С
ATOM	1332	CG2	VAL A	199	-17.369	46.686	118.322	1.00 50.88	C
ATOM	1333	N	TYR A		-19.242		118.734	1.00 22.51	N
ATOM	1334	CA	TYR A		-19.622		118.317	1.00 21.72	Ċ
									Č
ATOM	1335	С	TYR A		-18.416		117.848	1.00 23.34	C
ATOM	1336	0	TYR A	200	-17.535	53.419	118.652	1.00 19.31	0
MOTA	1337	CB	TYR A	200	-20.287	52.978	119.499	1.00 25.92	С
ATOM	1338	CG	TYR A		-20.828		119.240	1.00 27.65	С
			TYR A		-21.529		118.079	1.00 27.17	č
ATOM	1339								_
ATOM	1340	CD2			-20.698		120.204	1.00 31.21	Ċ
ATOM	1341	CE1	TYR A	200	-22.095	55.900	117.885	1.00 42.25	С
ATOM	1342	CE2	TYR A	200	-21.259	56.613	120.025	1.00 29.28	С
ATOM	1343	cz	TYR A		-21.957		118.863	1.00 37.99	Ċ
									ŏ
MOTA	1344	ОН	TYR A		-22.508		118.692	1.00 31.41	
MOTA	1345	N	SER A		-18.382		116.548	1.00 28.17	Ŋ
ATOM	1346	CA	SER A	201	-17.278	54.157	115.937	1.00 30.84	С
MOTA	1347	С	SER A		-17.668	55.572	115.552	1.00 28.96	C
ATOM	1348	ō	SER A		-18.321		114.531	1.00 33.52	ō
							114.688	1.00 26.64	č
ATOM	1349	CB	SER A		-16.743				
ATOM	1350	OG	SER A		-15.694		114.117	1.00 30.76	0
ATOM	1351	N	CYS A	202	-17.220		116.362	1.00 23.89	N
ATOM	1352	CA	CYS A		-17.526	57,923	116.149	1.00 21.53	С
ATOM	1353	Č.	CYS A		-16.596		115.165	1.00 21.15	č
								1.00 19.31	Ö
MOTA	1354	0	CYS A		-15.539		114.772		
ATOM	1355	CB	CYS A		-17.514		117.488	1.00 22.65	C
MOTA	1356	SG	CYS A	202	-18.438		118.743	1.00 42.79	S
ATOM	1357	N	GLU A		-17.030	59,822	114.758	1.00 16.28	N
ATOM	1358	CA	GLU A		-16.309		113.816	1.00 12.10	Ĉ
							114.456		č
ATOM	1359	C	GLU A		-16.364			1.00 7.30	Č
ATOM	1360	0	GLU A		-15.940		113.889	1.00 14.33	0
MOTA	1361	CB	GLU A	203	-17.036	60.667	112.460	1.00 3.31	С
ATOM	1362	CG	GLU A		-16.229		111.289	1.00 17.29	č
							109.957	1.00 28.70	č
MOTA	1363	CD	GLU A		-16.838				
MOTA	1364		GLU A		-16.898		109.647	1.00 41.61	0
ATOM	1365	OE2	GLU A	203	-17.272		109.222	1.00 46.00	0
ATOM	1366	N	TRP A		-16.901		115.669	1.00 3.31	N
MOTA	1367	CA	TRP A		-17.071		116.496	1.00 13.93	Ĉ
							116.392	1.00 20.85	č
ATOM	1368	С	TRP A	204	-15.931	04.231	110.372	1.00 20.83	·

ATOM	1369	0	TRP	A 204	-16.138	65.412 115.9	24 1.00	22.89	0
ATOM	1370	ČВ		A 204	-17.226	62.796 117.9		21.92	Ċ
ATOM	1371	ĊĞ		A 204	-17.538	63.837 118.9		21.15	Č
MOTA	1372			A 204	-17.489	65.194 118.8		20.49	č
ATOM	1373	_		A 204	-17.930	63.590 120.3		20.34	Ċ
ATOM	1374			A 204	-17.826	65.807 120.0		20.84	N
ATOM	1375			A 204	-18.102	64.846 120.9		25.47	Ċ
ATOM	1376			A 204	-18.153	62.424 121.0		15.62	č
ATOM	1377			A 204	-18.488	64.974 122.2		32.99	č
ATOM	1378			A 204	-18.538	62.551 122.4		21.84	č
ATOM	1379			A 204	-18.702	63.820 122.9		31.17	č
ATOM	1380	N		A 205	-14.705	63.919 116.7		27.07	N
MOTA	1381	CA		A 205	-13.530	64.801 116.7		22.40	Ċ
ATOM	1382	c		A 205	-13.351	65.527 115.4		12.76	č
ATOM	1383	ŏ		A 205	-13.259	66.750 115.4		3.31	ŏ
MOTA	1384	СВ		A 205	-12.370	63.848 117.0		32.69	č
ATOM	1385	CG		A 205	-12.998	62.723 117.7		38.48	č
ATOM	1386	CD		A 205	-14.290	62.529 117.0		37.95	č
ATOM	1387	N		A 206	-13.273	64.757 114.3		13.29	N
ATOM	1388	CA		A 206	-13.093	65.309 113.0		26.78	c c
MOTA	1389	c		A 206	-13.978	66.534 112.7		29.49	č
ATOM	1390	ŏ		A 206	-13.658	67.386 111.9		31.08	ŏ
ATOM	1391	СВ		A 206	-13.408	64.238 111.9		31.93	č
ATOM	1392	CG		A 206	-13.608	64.726 110.5		35.55	č
MOTA	1393			A 206	-12.286	65.202 109.9		44.15	č
ATOM	1394			A 206	-14.170	63.613 109.7		41.86	č
ATOM	1395	N		A 207	-15.087	66.636 113.5		33.41	Ň
MOTA	1396	CA		A 207	-15.958	67.769 113.2		42.82	ċ
ATOM	1397	c		A 201	-15.765	68.959 114.2		45.66	č
MOTA	1398	ŏ		A 207	-16.081	70.092 113.8		38.41	ŏ
ATOM	1399	СВ		A 201	-17.392	67.276 113.2		47.19	č
ATOM	1400	CG		A 207	-17.693	66.544 112.0		48.83	č
ATOM	1401			A 201	-17.773	67.236 110.8		48.74	č
ATOM	1402			A 201	-17.877	65.161 111.9		49.99	č
ATOM	1403	CEI		A 201	-18.031	66.582 109.6		47.79	č
ATOM	1404			A 20	-18.137	64.494 110.7		47.50	č
ATOM	1405	cz		A 207	-18.213	65.219 109.6		46.58	č
ATOM	1406	ОН		A 201	-18.482	64.602 108.4		52.10	ō
ATOM	1407	N.		A 208	-15.229	68.725 115.4		54.64	N
MOTA	1408	CA		A 208	-14.997	69.824 116.3		62.16	Ĉ
ATOM	1409	c		A 208	-13.958	70.772 115.7		62.53	č
ATOM	1410	ŏ		A 208	-14.064	71.980 115.9		67.29	ŏ
ATOM	1411	ČВ		A 208	-14.528	69.300 117.7		67.91	č
ATOM	1412	CG		A 208	-15.582	68.483 118.4		61.69	č
ATOM	1413	SD		A 208	-15.311	68.428 120.2		56.66	Š
ATOM	1414	CE		A 208	-15.639	70.115 120.6		59.92	c
ATOM	1415	N		A 209	-12.951	70.223 115.1		57.06	N
ATOM	1416	CA		A 209	-11.937	71.057 114.4		56.77	C
ATOM	1417	Ċ		A 209	-12.627	71.785 113.3		65.26	Ċ
ATOM	1418	ō		A 209	-13.511	71.236 112.7		63.65	ō
ATOM	1419	СB		A 209	-10.809	70.205 113.8		58.79	С
ATOM	1420	CG		A 209	-10.199	69.256 114.8		63.98	С
ATOM	1421	CD1		A 209	-10.758	68.117 115.3		68.80	С
ATOM	1422			A 209	-8.923	69.384 115.5		69.51	С
ATOM	1423	NE1		A 209	-9.915	67.524 116.2		75.45	N
ATOM	1424			A 209	-8.780	68.281 116.3		73.01	С
ATOM	1425	CE3		A 209	-7.886	70.324 115.4	427 1.00	77.58	С
ATOM	1426			A 209	-7.642	68.091 117.1	166 1.00	77.64	С
ATOM	1427	CZ3	TRP	A 209	-6.752	70.134 116.7	219 1.00	81.84	С
ATOM	1428			A 209		69.024 117.0		79.91	С
MOTA	1429	N		A 210		73.057 113.1	133 1.00	77.49	N
ATOM	1430	CA	PRO	A 210	-11.268	73.837 113.8		83.21	С
ATOM	1431	С	PRO	A -210	-11.939	74.940 114.6	688 1.00	79.01	С
ATOM	1432	0	PRO	A 210	-11.673	76.139 114.9		75.34	0
ATOM	1433	СВ	PRO	A 210	-10.420	74.399 112.7		90.90	С
ATOM	1434	CG	PRO	A 210	-11.471	74.755 111.7		92.14	С
MOTA	1435	CD		A 210	-12.462	73.592 111.		83.73	C
ATOM	1436	N		A 21	-12.815	74.512 115.9		76.58	N
ATOM	1437	CA		A 21	-13.545	75.420 116.4		73.52	C
ATOM	1438	С		A 21	-12.979	75.306 117.8		74.63	Ç
MOTA	1439	0		A 21	-12.983	76.273 118.6		77.50	0
MOTA	1440	CB		A 21:	-15.029	75.056 116.4		69.72	c
ATOM	1441	CG		A 21:	-15.570	74.891 115.0		67.85	c
ATOM	1442			A 21	-15.525	75.948 114.3		66.48	c
ATOM	1443			A 21		73.664 114.6		68.57	c
ATOM	1444			A 21		75.780 112.0		63.01	c
MOTA	1445			A 21	-16.478	73.494 113.		66.32	C
ATOM	1446	CZ		A 21	-16.420	74.556 112.4		58.64	C
MOTA	1447	N		A 212	-12.485	74.122 118.2		73.94	N C
MOTA	1448	CA		A 213		73.900 119.5 72.470 119.6		72.71 67.26	Č
MOTA	1449	С	OLN	A 21	-11.416	12.410 113.0	U-15 1.00	07.20	·

ATOM	1450	O GLN	A 212	-12.089	71.534 119.197	1.00 66.79	o
ATOM	1451		A 212	-12.874	74.241 120.638	1.00 82.79	č
ATOM	1452		A 212	-14.246	73.590 120.537	1.00 94.62	č
MOTA	1453	CD GLN	A 212	-15.224	74.107 121.597	1.00101.94	C
MOTA	1454	OE1 GLN		-15.575	75.280 121.596	1.00107.83	0
MOTA	1455	NE2 GLN		-15.648	73.235 122.508	1.00101.67	N
MOTA	1456		A 213	-10.241	72.313 120.235	1.00 66.10	N
ATOM	1457		A 213	-9.673	71.002 120.431	1.00 72.81	Ç
MOTA	1458		A 213	-10.686	70.246 121.291	1.00 67.35	Ğ
ATOM	1459		A 213	-11.203	70.780 122.264	1.00 68.84	0
ATOM	1460		A 213	-8.321	71.121 121.147	1.00 86.07	C
MOTA MOTA	1461 1462		A 213 A 213	-7.531 -8.194	72.359 120.742	1.00100.84	C
ATOM	1463		A 213	-7.474	73.597 121.312 74.868 120.947	1.00110.24 1.00115.97	C
ATOM	1464		A 213	-8.130	76.003 121.647	1.00113.67	N
ATOM	1465		A 214	-10.992	68.994 120.925	1.00 63.52	N
ATOM	1466		A 214	-11.951	68.140 121.643	1.00 65.13	Ċ
MOTA	1467		A 214	-11.464	67.635 122.998	1.00 64.40	č
ATOM	1468	O PRO	A 214	-10.277	67.648 123.269	1.00 66.33	0
MOTA	1469	CB PRO	A 214	-12.171	66.984 120.666	1.00 72.41	С
ATOM	1470	CG PRO	A 214	-11.718	67.518 119.322	1.00 65.19	С
MOTA	1471		A 214	-10.519	68.333 119.694	1.00 61.91	С
MOTA	1472		A 215	-12.387	67.220 123.854	1.00 65.67	N
ATOM	1473		A 215	-11.989	66.670 125.138	1.00 67.56	Č
MOTA	1474		A 215	-11.969	65.171 124.904	1.00 62.72	C
ATOM	1475 1476		A 215	-12.946	64.479 125.173	1.00 59.58	0
ATOM ATOM	1477		A 215 A 215	-12.998 -12.635	67.014 126.235 66.389 127.567	1.00 81.52 1.00 93.94	C
ATOM	1478	OD1 ASN		-11.640	65.666 127.656	1.00 97.55	o
ATOM	1479	ND2 ASN		-13.421	66.667 128.608	1.00106.11	N
ATOM	1480		A 216	-10.852	64.681 124.381	1.00 58.40	N
MOTA	1481		A 216	-10.702	63.267 124.061	1.00 51.54	Ċ
MOTA	1482		A 216	-11.016	62.331 125.217	1.00 52.52	Ċ
MOTA	1483		A 216	-11.460	61.197 125.006	1.00 46.44	0
ATOM	1484		A 216	-9.285	62.987 123.556	1.00 43.79	С
MOTA	1485		A 216	-9.029	63.400 122.122	1.00 33.73	С
ATOM	1486	CD1 TYR		-9.687	62.772 121.064	1.00 33.94	С
ATOM	1487	CD2 TYR		-8.116	64.415 121.814	1.00 28.64	C
ATOM	1488	CE1 TYR		-9.439	63.146 119.726	1.00 22.17	C
ATOM ATOM	1489 1490	CE2 TYR		-7.868	64.795 120.477	1.00 22.68	c
ATOM	1491		A 216 A 216	-8.533 -8.293	64.156 119.440 64.523 118.125	1.00 19.76 1.00 20.60	C O
ATOM	1492		A 217	-10.769	62.788 126.440	1.00 20.00	N
ATOM	1493		A 217	-11.046	61.952 127.603	1.00 50.03	Č
ATOM	1494		A 217	-12.546	61.764 127.630	1.00 49.02	č
ATOM	1495		A 217	-13.045	60.706 128.003	1.00 56.07	ŏ
MOTA	1496	CB THR	A 217	-10.591	62.623 128.909	1.00 51.67	c
ATOM	1497	OG1 THR	A 217	-9.252	63.112 128.750	1.00 59.45	0
ATOM	1498	CG2 THR		-10.606	61.618 130.053	1.00 50.17	С
ATOM	1499		A 218	-13.251	62.810 127.217	1.00 44.02	N
ATOM	1500		A 218	-14.702	62.804 127.151	1.00 38.09	C
ATOM	1501		A 218	-15.095 -15.626	61.779 126.101 60.714 126.408	1.00 30.35	C
ATOM ATOM	1502 1503		A 218 A 218	16 102	64.196 126.747	1.00 31.42 1.00 45.80	0 C
ATOM	1504		A 218	-15.162	64.351 126.544	1.00 56.73	c
ATOM	1505		A 218	-15.162 -16.669 -17.145 -17.061	65.729 126.966	1.00 62.81	c
ATOM	1506	OE1 GLU	A 218	-17.061	66.034 128.180	1.00 64.60	ŏ
ATOM		OE2 GLU	A 218	-17.591	66.506 126.093		ŏ
MOTA	1508		A 219	-14.804	62.116 124.854	1.00 20.92	N
MOTA	1509		A 219	-15.092	61.260 123.711	1.00 16.81	С
MOTA	1510		A 219	-14.830	59.784 123.978	1.00 19.92	C
ATOM	1511		A 219	-15.674	58.938 123.685	1.00 26.14	0
ATOM	1512		A 219	-14.233	61.659 122.517	1.00 18.69	c c
ATOM	1513	CG1 ILE		-14.460	63.136 122.189	1.00 28.40	C
ATOM	1514 1515	CG2 ILE		-14.546	60.759 121.343	1.00 3.31	c c
ATOM ATOM	1516	CD1 ILE		-13.861 -13.645	63.582 120.873	1.00 35.19 1.00 22.71	N
ATOM	1517		A 220 A 220	-13.250	59.488 124.511 58.121 124.815	1.00 22.71	C
ATOM	1518		A 220	-14.251	57.426 125.723	1.00 36.46	c
ATOM	1519		A 220	-14.291	56.202 125.778	1.00 41.29	0
ATOM	1520		A 220	-11.862	58.100 125.458	1.00 34.29	С
MOTA	1521		A 220	-11.602	56.838 126.251	1.00 44.46	ċ
MOTA	1522		A 220	-10.137	56.579 126.435	1.00 58.36	c c
MOTA	1523	NE ARG	A 220	-9.873	55.151 126.320	1.00 81.14	N
MOTA	1524		A 220	-8.660	54.612 126.325	1.00 95.08	C
ATOM	1525	NH1 ARG		-7.589	55.383 126.442	1.00100.76	N
MOTA	1526	NH2 ARG		-8.519	53.300 126.202	1.00102.37	N
ATOM ATOM	1527 1528		A 221 A 221	-15.054 -16.063	58.205 126.441 57.643 127.334	1.00 38.90 1.00 44.66	N C
ATOM	1529		A 221	-17.346	57.461 126.563	1.00 42.86	c
ATOM	1530		A 221	-18.404	57.257 127.147	1.00 46.12	ŏ
	_			==			_

MOTA	1531	CB G	LN A	221	-16.354	58.583 128.493	1.00 51.89	C
ATOM	1532		LN A					
					-15.174	58.935 129.342		C
MOTA	1533	CD G	LN A	221	-15.591	59.700 130.569	1.00 74.55	C
ATOM	1534	OE1 G	LN A	221	-16.235	60.746 130.476		0
ATOM	1535							
		NE2 G			-15.230	59.182 131.73		N
ATOM	1536	N T	YR A	222	-17.247	57.542 125.244	1.00 45.18	N
MOTA	1537	CA T	YR A	222	-18.415	57.416 124.389	1.00 48.79	C
MOTA	1538		YR A		-18.160	56.677 123.087		C
ATOM	1539	O T	YR A	222	-19.099	56.411 122.326	1.00 52.15	0
MOTA	1540		YR A		-18.957	58.805 124.062		Ċ
ATOM	1541		YR A		-19.687	59.469 125.197	1.00 54.32	C
ATOM	1542	CD1 T	YR A	222	-20.824	58.885 125.751	1.00 63.31	C
MOTA	1543	CD2 T			-19.280	60.707 125.680		Ċ
ATOM	1544	CE1 T			-21.540	59.521 126.747	1.00 65.52	C
ATOM	1545	CE2 T	YR A	222	-19.990	61.353 126.681	1.00 68.64	C
ATOM	1546		YR A		-21.120	60.756 127.205		Č
ATOM	1547		YR A		-21.847	61.409 128.164	1.00 59.66	0
ATOM	1548	N C	YS A	223	-16.905	56.341 122.806	1.00 47.24	N
MOTA	1549		YS A	223	-16.600	55.672 121.555		Ċ
MOTA	1550		YS A		-15.539	54.605 121.640	1.00 43.74	C
MOTA	1551	O C.	YS A	223	-14.649	54.652 122.490	1.00 48.31	.0
MOTA	1552		YS A		-16.183	56.714 120.538		Ċ
MOTA	1553		YS A		-17.410	58.054 120.464		S
MOTA	1554	N A	SN A	224	-15.644	53.636 120.741	. 1.00 38.10	N
ATOM	1555	CA A	SN A	224	-14.684	52.552 120.681		С
MOTA	1556		SN A		-13.505	53.023 119.840		C
ATOM	1557	O A:	SN A	224	-12.395	52.498 119.939	1.00 33.20	0
MOTA	1558	CB A	SN A	224	-15.367	51.323 120.104	1.00 35.64	C
ATOM								
	1559		SN A		-16.398	50.759 121.056		C
ATOM	1560	OD1 A	SN A	224	-17.510	50.428 120.669	1.00 32.93	0
ATOM	1561	ND2 AS	SN A	224	-16.026	50.646 122.323	1.00 23.40	N
ATOM	1562		IS A		-13.772	54.029 119.014		N
ATOM	1563	CA H	IS A	225	-12.771	54.677 118.177	1.00 37.53	С
ATOM	1564	C H:	IS A	225	-13.418	55.766 117.343	1.00 40.70	С
ATOM	1565		IS A			55.649 116.892		
					-14.551			0
MOTA	1566	CB H	IS A	225	-11.966	53.679 117.322	1.00 37.41	C
ATOM	1567	CG H	IS A	225	-12.763	52.542 116.770	1.00 35.26	Ċ
ATOM	1568	ND1 H			-13.722	52.703 115.793		N
ATOM	1569	CD2 H	15 A	225	-12.696	51.214 117.019	1.00 31.85	Ç
ATOM	1570	CE1 H	IS A	225	-14.208	51.521 115.464	1.00 26.70	С
ATOM	1571	NE2 H			-13.602	50.601 116.193		N
MOTA	1572		RP A		-12.665	56.839 117.166	1.00 40.42	N
ATOM	1573	CA TI	RP A	226	-13.114	58.039 116.477	1.00 36.10	С
ATOM	1574		RP A		-12.185	58.503 115.343		č
MOTA	1575		RP A		-10.994	58.189 115.340	1.00 37.97	0
ATOM	1576	CB TI	RP A	226	-13.201	59.127 117.530	1.00 26.81	С
ATOM	1577	CG TI	RP A	226	-11.949	59.110 118.387		Ċ
ATOM	1578	CD1 T						
					-10.738	59.675 118.081		С
ATOM	1579	CD2 TE	RP A	226	-11.746	58.383 119.613	1.00 33.48	С
ATOM	1580	NE1 TE	RP A	226	-9.802	59.344 119.032	1.00 31.17	N
ATOM	1581	CE2 T			-10.394	58.556 119.984		
								C
ATOM	1582	CE3 TF	RP A	226	-12.575	57.607 120.433	1.00 35.17	С
ATOM	1583	CZ2 TF	RP A	226	-9.850	57.972 121.132	1.00 27.64	С
ATOM	1584	CZ3 TF			-12.030	57.027 121.576		č
ATOM	1585	CH2 TF			-10.681	57.219 121.914	1.00 28.55	C
MOTA	1586	N AF	RG A	227	-12.735	59.254 114.389	1.00 27.57	N
ATOM	1587	CA AF	RG A	227	-11.955	59.790 113.273	1.00 30.76	С
ATOM	1588		RG A					
					-11.303	61.097 113.696		C
ATOM	1589	O AF	RG A	227	-11.854	61.822 114.511	1.00 36.24	0
ATOM	1590	CB AF	RG A	227	-12.861	60.057 112.080	1.00 32.55	C
ATOM	1591		RG A		-13.215	58.830 111.283		Ċ
MOTA	1592		RG A		-12.012	58.339 110.509		С
ATOM	1593	NE AF	RG A	227	-11.628	59.262 109.450	1.00 31.33	N
ATOM	1594		RG A		-12.398	59.555 108.410		С
ATOM	1595	NH1 AF			-13.593	58.999 108.294		N
ATOM	1596	NH2 AF	RG A	227	-11.970	60.395 107.481	1.00 45.28	N
ATOM	1597	N AS	SN A	228	-10.137	61.406 113.145	1.00 34.78	N
ATOM	1598		SN A		-9.447	62.639 113.505		c c
MOTA	1599		SN A		-9.193	63.528 112.311		С
MOTA	1600	O AS	SN A	228	-9.435	64.727 112.351	1.00 40.12	0
MOTA	1601		SN A		-8.099	62.344 114.176		č
MOTA	1602		SN A		-8.245	61.660 115.525		C
MOTA	1603	OD1 AS			-9.082	62.038 116.342		0
ATOM	1604	ND2 AS			-7.413	60.654 115.769		N
ATOM	1605		iE A		-8.699	62.929 111.241	1.00 45.11	N
MOTA	1606		IE A		-8.377	63.681 110.038		С
MOTA	1607	C Ph	IE A	229	-9.375	63.406 108.920	1.00 37.97	С
MOTA	1608		IE A		-10.218	62.516 109.034		ō
ATOM	1609		iE A		-6.964	63.315 109.571		č
							1.00 38.01	Č
MOTA	1610		IE A		-6.359	64.315 108.641	1.00 31.14	C
MOTA	1611	CD1 PF	IE A	229	-6.097	65.610 109.077	1.00 29.66	С

MOTA	1612 CD2	PHE A 229.	-6.081	63.973 107.319	1.00 38.07	С
ATOM		PHE A 229	-5.568	66.552 108.212	1.00 45.65	č
ATOM		PHE A 229	-5.553	64.906 106.440	1.00 39.87	č
ATOM	1615 CZ	PHE A 229				
MOTA	1616 N		-5.297	66.201 106.886	1.00 44.87	C
		ALA A 230	-9.266	64.176 107.841	1.00 40.67	N
ATOM	1617 CA	ALA A 230	-10.136	64.037 106.673	1.00 45.66	С
MOTA	1618 C	ALA A 230	-10.186	62.599 106.153	1.00 43.65	
ATOM	1619 0	ALA A 230	-9.459	61.738 106.645	1.00 40.62	0
MOTA	1620 CB	ALA A 230	-9.643	64.961 105.563	1.00 50.69	С
ATOM	1621 N	ASP A 231	-11.044	62.336 105.166	1.00 45.95	N
ATOM	1622 CA	ASP A 231	-11.106	60.995 104.594	1.00 46.27	
ATOM		ASP A 231	-9.771	60.655 103.974	1.00 39.23	č
ATOM		ASP A 231	-8.800	61.402 104.111	1.00 33.23	
ATOM		ASP A 231			1.00 47.23	Ü
			-12.164	60.888 103.523	1.00 57.49	Ç
ATOM		ASP A 231	-13.526	60.822 104.092	1.00 65.88	С
MOTA		ASP A 231	-13.665	60.206 105.166	1.00 69.45	0
MOTA		ASP A 231	-14.455	61.372 103.466	1.00 71.23	0
MOTA	1629 N	ILE A 232	-9.721	59.540 103.265	1.00 24.74	N
MOTA	1630 CA	ILE A 232	-8.466	59.128 102.678	1.00 24.77	С
ATOM	1631 C	ILE A 232	-8.611	58.666 101.230	1.00 33.28	Ċ
ATOM		ILE A 232	-9.423	57.789 100.935	1.00 40.10	ŏ
ATOM		ILE A 232	-7.837	58.019 103.561	1.00 25.18	Č
MOTA		ILE A 232	-6.497	57.550 102.984	1.00 23.10	Č
MOTA		ILE A 232			1.00 18.54	Č
ATOM			-8.824	56.876 103.709	1.00 33.13	۲
		ILE A 232	-5.676	56.721 103.976	1.00 18.15	Ľ
MOTA		ASP A 233	-7.826	59.283 100.339	1.00 40.33	N
MOTA		ASP A 233	-7.814	58.967 98.907	1.00 38.66	С
ATOM		ASP A 233	-6.932	57.755 98.685	1.00 33.49	С
MOTA	1640 O	ASP A 233	-6.180	57.368 99.558	1.00 41.14	. 0
MOTA	1641 CB	ASP A 233	-7.191	60.106 98.088	1.00 49.03	C
ATOM	1642 CG	ASP A 233	-7.943	61.412 98.204	1.00 69.46	Ċ
MOTA		ASP A 233	-9.109	61.479 97.753	1.00 80.91	ō
ATOM		ASP A 233	-7.349	62.372 98.745	1.00 76.24	ŏ
ATOM		ASP A 234	-7.012	57.157 97.510	1.00 76.24	U U
MOTA		ASP A 234	-6.143		1.00 27.40	N
				56.037 97.208	1.00 28.65	Ċ
ATOM		ASP A 234	-4.904	56.746 96.662	1.00 29.50	С
ATOM		ASP A 234	-4.595	56.662 95.462	1.00 28.14	0
ATOM		ASP A 234	-6.777	55.147 96.141	1.00 31.14	С
ATOM		ASP A 234	-5.995	53.879 95.922	1.00 35.74	С
MOTA	1651 OD1	ASP A 234	-5.181	53.528 96.808	1.00 33.60	0
ATOM	1652 OD2	ASP A 234	-6.196	53.219 94.884	1.00 38.85	0
MOTA	1653 N	SER A 235	-4.213	57.458 97.556	1.00 27.77	N
ATOM	1654 CA	SER A 235	-3.032	58.242 97.187	1.00 27.25	Ċ
ATOM		SER A 235	-1.960	58.300 98.253	1.00 24.27	č
ATOM		SER A 235	-2.235	58.128 99.444	1.00 20.06	0
ATOM		SER A 235	-3.457	59.674 96.880	1.00 36.86	0
ATOM		SER A 235	-4.172		1.00 30.00	C
ATOM				60.234 97.980	1.00 27.30	0
		TRP A 236	-0.733	58.573 97.831	1.00 19.59	N
MOTA		TRP A 236	0.365	58.683 98.787	1.00 22.03	С
ATOM		TRP A 236	0.169	59.972 99.601	1.00 23.19	C
MOTA		TRP A 236	0.300	59.981 100.834	1.00 27.64	0
MOTA		TRP A 236	1.698	58.719 98.041	1.00 23.81	С
MOTA		TRP A 236	2.952	58.843 98.887	1.00 15.41	С
ATOM	1665 CD1 1	TRP A 236	4.090	59.515 98.548	1.00 14.82	С
MOTA	1666 CD2 1	TRP A 236	3.206	58.260 100.180	1.00 20.27	С
ATOM	1667 NE1 1	TRP A 236	5.031	59.391 99.538	1.00 13.94	N
MOTA	1668 CE2 1	TRP A 236	4.519	58.627 100.552	1.00 16.04	Ċ
MOTA	1669 CE3 1	TRP A 236	2.454	57.465 101.056	1.00 31.69	č
ATOM		TRP A 236	5.098			č
ATOM		TRP A 236	3.034	57.066 102.266	1.00 29.69	č
ATOM	1672 CH2 1	TRP A 236	4.345		1.00 25.33	Č
ATOM				57.452 102.602		C
		LYS A 237	-0.167	61.053 98.902	1.00 25.83	N
ATOM		LYS A 237	-0.396	62.347 99.532	1.00 34.83	c
ATOM		LYS A 237	-1.338	62.218 100.724	1.00 40.41	С
ATOM		LYS A 237	-0.959	62.489 101.866	1.00 44.29	0
MOTA		LYS A 237	-0.990	63.316 98.517	1.00 41.22	С
MOTA		LYS A 237	-1.285	64.702 99.054	1.00 50.27	С
MOTA	1679 CD I	LYS A 237	-1.854	65.592 97.958	1.00 66.37	Ċ
MOTA		LYS A 237	-2.078	67.010 98.448	1.00 75.77	Č
MOTA		LYS A 237	-2.520	67.895 97.341	1.00 85.31	N
ATOM		SER A 238	-2.565	61.793 100.454	1.00 47.13	N N
ATOM		SER A 238	-3.561	61.625 101.496	1.00 49.36	ć
ATOM		SER A 238	-2.979	60.909 102.716	1.00 41.87	č
MOTA		SER A 238	-3.281	61.251 103.865	1.00 43.11	o
ATOM		SER A 238	-4.733	60.827 100.954	1.00 58.97	Č
MOTA		SER A 238	-9.733 -5.767	60.730 101.922	1.00 58.97	
ATOM						0
ATOM		ILE A 239	-2.130	59.919 102.478	1.00 28.63	N
ATOM		ILE A 239	-1.538	59.205 103.596	1.00 25.25	C
ATOM		ILE A 239	-0.518	60.068 104.307	1.00 21.50	c
		ILE A 239	-0.537	60.181 105.535	1.00 16.28	0
ATOM	1692 CB I	ILE A 239	-0.905	57.882 103.129	1.00 22.82	С

						_
ATOM	1693	CG1 ILE A 23		56.813 103.085	1.00 30.64	C
MOTA	1694	CG2 ILE A 23	9 0.247	57.481 104.031	1.00 18.42	C
MOTA	1695	CD1 ILE A 23	9 -1.507	55.390 103.020	1.00 32.95	C
MOTA	1696	N LYS A 24			1.00 20.19	Ñ
MOTA	1697	CA LYS A 24				Ċ
					1.00 27.65	
ATOM	1698	C LYS A 24		62.543 105.075	1.00 35.03	C
ATOM	1699	O LYS A 24		62.633 106.249	1.00 40.16	0
ATOM	1700	CB LYS A 24	0 2.158		1.00 36.93	C
ATOM	1701	CG LYS A 24			1.00 41.89	Č
ATOM	1702					_
		CD LYS A 24		62.019 100.851	1.00 50.69	C
MOTA	1703	CE LYS A 24		63.097 101.229	1.00 56.56	C
MOTA	1704	NZ LYS A 24	0 4.883	63.829 100.039	1.00 68.08	N
ATOM	1705	N SER A 24			1.00 32.20	N
ATOM	1706	CA SER A 24				Ċ
				64.278 105.406	1.00 33.89	
ATOM	1707	C SER A 24		63:692 106.731	1.00 30.55	C
MOTA	1708	O SER A 24	1 -1.210	64.290 107.792	1.00 22.28	0
ATOM	1709	CB SER A 24	1 -2.050	64.932 104.628	1.00 38.13	С
MOTA	1710	OG SER A 24		63.982 104.200	1.00 52.37	ŏ
ATOM	1711	N ILE A 24				
				62.529 106.673	1.00 25.28	N
ATOM	1712	CA ILE A 24		61.888 107.884	1.00 21.26	C
ATOM	1713	C ILE A 24	2 -1.444	61.603 108.880	1.00 25.16	С
MOTA	1714	O ILE A 24	2 -1.552	61.896 110.084	1.00 25.43	0
MOTA	1715	CB ILE A 24		60.569 107.546	1.00 14.21	Č
MOTA	1716	CG1 ILE A 24		60.893 107.175		
					1.00 17.53	C
ATOM	1717	CG2 ILE A 24		59.615 108.730	1.00 13.13	Ç
ATOM	1718	CD1 ILE A 24		59.668 106.946	1.00 19.53	С
MOTA	1719	N LEU A 24	3 -0.350	61.033 108.392	1.00 18.34	N
MOTA	1720	CA LEU A 24		60.779 109.284	1.00 10.66	C
ATOM	1721	C LEU A 24		62.133 109.817	1.00 19.50	Č
ATOM	1722	O LEU A 24				
				62.404 111.015	1.00 21.45	0
ATOM	1723	CB LEU A 24		60.159 108.527	1.00 12.02	С
MOTA	1724	CG LEU A 24	3 1.811	58.654 108.356	1.00 7.19	С
MOTA	1725	CD1 LEU A 24	3 2.998	58.195 107.559	1.00 3.85	С
ATOM	1726	CD2 LEU A 24		57.975 109.709	1.00 13.48	č
ATOM	1727	N ASP A 24		62.979 108.893		
					1.00 17.56	N
ATOM	1728	CA ASP A 24		64.329 109.210	1.00 19.63	С
MOTA	1729	C ASP A 24		64.987 110.247	1.00 20.63	С
ATOM	1730	O ASP A 24	1.625	65.813 111.053	1.00 17.63	0
MOTA	1731	CB ASP A 24		65.194 107.957	1.00 24.06	č
ATOM	1732	CG ASP A 24		64.850 107.017		
					1.00 30.13	Ç
ATOM	1733	OD1 ASP A 24		64.624 107.499	1.00 37.52	0
ATOM	1734	OD2 ASP A 24		64.832 105.787	1.00 30.05	0
MOTA	1735	N TRP A 24	-0.091	64.615 110.207	1.00 14.39	N
ATOM	1736	CA TRP A 24	-1.068	65.168 111.111	1.00 13.88	Ċ
ATOM	1737	C TRP A 24		64.455 112.452	1.00 16.86	č
ATOM	1738					
				65.091 113.506	1.00 20.50	0
ATOM	1739	CB TRP A 24		65.056 110.493	1.00 17.62	C
MOTA	1740	CG TRP A 24	-3.462	65.705 111.336	1.00 34.54	٠c
MOTA	1741	CD1 TRP A 24!	-3.851	67.017 111.293	1.00 41.20	С
ATOM	1742	CD2 TRP A 245		65.118 112.458	1.00 31.61	č
ATOM	1743	NEI TRP A 24		67.283 112.329		
ATOM	1744				1.00 47.44	N
		CE2 TRP A 24		66.135 113.060	1.00 34.63	С
ATOM	1745	CE3 TRP A 249		63.828 113.018	1.00 31.06	С
ATOM	1746	CZ2 TRP A 245	-5.690	65.902 114.200	1.00 35.09	С
ATOM	1747	CZ3 TRP A 245	-4.925	63.597 114.147	1.00 36.08	С
ATOM	1748	CH2 TRP A 245		64.630 114.726	1.00 37.13	č
ATOM	1749	N THR A 240		63.134 112.415	1.00 17.45	N
ATOM	1750					
		CA THR A 246		62.355 113.643	1.00 11.72	C
ATOM	1751	C THR A 246	0.267	62.518 114.309	1.00 13.47	С
ATOM	1752	O THR A 246	0.421	62.340 115.518	1.00 3.31	0
MOTA	1753	CB THR A 246		60.889 113.348	1.00 13.70	С
ATOM	1754	OG1 THR A 246		60.607 113.651	1.00 22.35	ŏ
MOTA	1755	CG2 THR A 246		59.992 114.151	1.00 22.33	
ATOM						C
	1756	N SER A 247		62.852 113.501	1.00 19.43	N
ATOM	1757	CA SER A 247		63.070 113.998	1.00 25.96	С
MOTA	1758	C SER A 247		64.327 114.873	1.00 31.04	С
MOTA	1759	O SER A 247		64.305 116.069	1.00 29.04	Ō
MOTA	1760	CB SER A 247		63.286 112.803	1.00 19.11	č
ATOM	1761	OG SER A 247		63.592 113.220	1.00 40.79	ò
MOTA	1762					
				65.411 114.224	1.00 39.78	N
ATOM	1763	CA PHE A 248		66.757 114.772	1.00 45.15	С
MOTA	1764	C PHE A 248		66.960 115.792	1.00 39.54	С
ATOM	1765	O PHE A 248		68.087 116.041	1.00 44.71	Ō
MOTA	1766	CB PHE A 248		67.691 113.594	1.00 64.18	ř
ATOM	1767	CG PHE A 248		69.126 113.879	1.00 77.73	ž
ATOM	1768	CD1 PHE A 248		69.573 114.137		Č
					1.00 86.07	Ç
MOTA	1769	CD2 PHE A 248		70.049 113.788	1.00 80.31	С
ATOM	1770	CE1 PHE A 248		70.924 114.298	1.00 92.63	С
ATOM	1771	CE2 PHE A 248		71.400 113.946	1.00 84.15	c c c c c
MOTA	1772	CZ PHE A 248		71.844 114.195	1.00 93.81	č
MOTA	1773	N ASN A 249		65.888 116.401	1.00 35.73	N
	-		00			N

ATOM	1774	CA	ASN	Δ	249	-0.611	66.033	117.355	1.00 34.50	С
						-0.607				
ATOM	1775	С	ASN					118.504	1.00 40.42	С
ATOM	1776	0	ASN	Α	249	-1.376	65.203	119.445	1.00 42.06	0
MOTA	1777	CB	ASN	Α	249	-1.944	65.922	116.633	1.00 25.27	С
			ASN			-2.435		116.144	1.00 27.53	č
MOTA	1778	CG								
ATOM	1779	OD1	ASN	Α	249	-2.504		116.914	1.00 34.54	0
MOTA	1780	ND2	ASN	Α	249	-2.782	67.321	114.863	1.00 23.24	N
ATOM	1781	N	GLN			0.256	64 053	118.429	1.00 43.93	N
MOTA	1782	CA	GLN			0.338		119.472	1.00 45.21	С
MOTA	1783	С	GLN	Α	250	0.044	63.578	120.876	1.00 45.89	С
ATOM	1784	ō	GLN			-0.597		121.674	1.00 46.33	0
										č
MOTA	1785	CB	GLN			1.710		119.429	1.00 49.33	С
MOTA	1786	CG	GLN	Α	250	2.754	63.146	118.653	1.00 56.41	С
MOTA	1787	CD	GLN			3.999	62.330	118.422	1.00 67.52	С
									1.00 64.03	ō
MOTA	1788		GLN			3.934		117.884		
ATOM	1789	NE2	GLN	Α	250	5.145	62.868	118.826	1.00 73.52	N
ATOM	1790	N	GLU	Α	251	0.497	64.795	121.176	1.00 46.19	N
ATOM	1791	CA	GLU			0.255		122.490	1.00 53.10	c
										č
MOTA	1792	С	GLU			-1.149		122.981	1.00 55.27	
MOTA	1793	0	GLU	Α	251	-1.327	64.466	124.031	1.00 63.00	0
ATOM	1794	CB	GLU	Α	251	0.433	66.908	122.450	1.00 61.86	С
ATOM	1795	CG	GLU			1.837		122.738	1.00 77.46	Ċ
ATOM	1796	CD	GLU	Α	251	2.837		121.742	1.00 89.72	С
ATOM	1797	OE1	GLU	Α	251	3.019	65.618	121.679	1.00 97.55	0
MOTA	1798		GLU			3.443	67.666	121.017	1.00 95.81	0
						-2.143			1.00 50.90	N
MOTA	1799	N	ARG					122.201		
ATOM	1800	CA	ARG	Α	252	-3.541	65.290	122.567	1.00 50.56	С
ATOM	1801	С	ARG	Α	252	-4.116	63.899	122.362	1.00 46.98	С
ATOM	1802	Ō	ARG			-4.856		123.215	1.00 53.85	0
ATOM	1803	CB	ARG	А	252	-4.435		121.806	1.00 57.95	С
ATOM	1804	CG	ARG	Α	252	-4.082	67.703	121.974	1.00 73.90	С
ATOM	1805	CD	ARG			-5.043	68.562	121.193	1.00 91.08	С
	1806					-4.553		121.068	1.00109.12	N
ATOM		NE	ARG							
MOTA	1807	CZ	ARG			-3.422		120.452	1.00117.35	С
ATOM	1808	NH1	ARG	Α	252	-2.652	69.335	119.898	1.00121.60	N
MOTA	1809	NH2	ARG			-3.056	71.540	120.391	1.00122.11	N
			ILE			-3.789		121.240	1.00 34.95	N
ATOM	1810	N								
MOTA	1811	CA	ILE	Α	253	-4.349		120.939	1.00 26.82	С
ATOM	1812	С	ILE	A	253	-3.613	60.720	121.402	1.00 34.17	Ċ
MOTA	1813	0	ILE	Δ	253	-4.170	59 911	122.146	1.00 35.29	0
						-4.590		119.447	1.00 12.97	č
MOTA	1814	CB	ILE							Č
MOTA	1815		ILE			-3.310		118.687	1.00 3.31	Ċ
MOTA	1816	CG2	ILE	Α	253	-5.712	62.764	119.039	1.00 24.79	С
ATOM	1817		ILE			-3.460		117.175	1.00 14.82	С
						-2.374		120.949	1.00 42.48	Ň
ATOM	1818	N	VAL							
MOTA	1819	CA	VAL	Α	254	-1.559		121.286	1.00 51.32	С
ATOM	1820	С	VAL	Α	254	-1.798	58.828	122.688	1.00 53.95	С
MOTA	1821	0	VAL			-1.683		122.922	1.00 55.92	0
						-0.049		121.164	1.00 49.29	Č
ATOM	1822	СВ	VAL							
MOTA	1823	CG1	VAL	А	254	0.465		122.444	1.00 52 01	С
MOTA	1824	CG2	VAL	Α	254	0.717	58.427	120.872	1.00 50.05	С
ATOM	1825	N	ASP	Δ	255	-2.136	59.721	123.609	1.00 56.09	N
								125.010	1.00 63.32	Ċ
ATOM	1826	ÇA	ASP			-2.362				
ATOM	1827	С	ASP	Α	255	-3.674	58.653	125.344	1.00 58.30	С
ATOM	1828	0	ASP	Α	255	-3.650	57.535	125.865	1.00 61.53	. 0
MOTA	1829	CB	ASP			-2.273	60 672	125.834	1.00 81.31	С
								127.163	1.00 92.58	č
ATOM	1830	CG	ASP			-1.609				
MOTA	1831		ASP			-1.664		128.007	1.00103.11	0
ATOM	1832	OD2	ASP	Α	255	-1.028	59.369	127.355	1.00 95.27	0
ATOM	1833	N	VAL			-4.810		125.060	1.00 47.34	N
									1.00 26.26	č
ATOM	1834	CA	VAL			-6.124		125.339		
ATOM	1835	С	VAL	Α	256	-6.393	57.401	124.612	1.00 20.16	С
ATOM	1836	0	VAL	А	256	-7.515	56.896	124.638	1.00 21.60	0
ATOM	1837	СВ	VAL			-7.236		124.966	1.00 17.99	С
								126.003		Ž.
ATOM	1838		VAL			-7.333			1.00 15.54	Č
ATOM	1839	CG2	VAL	Α	256	-6.943		123.608	1.00 11.70	Ċ
ATOM	1840	N	ALA			-5.365	56.852	123.968	1.00 21.31	N
ATOM	1841	CA	ALA			-5.478		123.238	1.00 24.74	С
								124.143	1.00 28.46	č
ATOM	1842	C	ALA			-5.261				
MOTA	1843	0	ALA	Α	257	-4.374		125.000	1.00 34.08	0
ATOM	1844	CB	ALA			-4.477	55.578	122.112	1.00 30.69	С
ATOM	1845	N	GLY			-6.071		123.935	1.00 27.17	N
ATOM	1846	CA	GLY			-5.958		124.731	1.00 34.38	C
ATOM	1847	С	GLY			-7.229		124.602	1.00 39.07	Ċ
ATOM	1848	0	GLY	Α	258	-8.186	51.801	123.994	1.00 46.72	0
ATOM	1849	N	PRO			-7.274		125.164	1.00 41.39	N
	1850				259			125.103	1.00 37.99	Ċ
ATOM		CA				-8.450				Ž
MOTA	1851	С			259	-9.781		125.261	1.00 38.04	c
MOTA	1852	0	PRO	Α	259	-9.930		126.124	1.00 37.32	0
ATOM	1853	CB			259	-8.191		126.230	1.00 41.03	С
ATOM	1854	CG			259	-6.731		126.112	1.00 44.48	Č
	-037			• •		3.732				•

MOTA	1855	CD	PRO	A	259	-6.202	49 488	125.940	1.00 4	7 07	С
ATOM	1856	N			260	-10.749		124.424	1.00 3		
						-12.057					N
MOTA	1857	CA			260			124.500	1.00 3		c
MOTA	1858	C			260	-12.173		123.560	1.00 2		Č
MOTA	1859	0			260	-13.188		122.896	1.00 1		0
MOTA	1860	N			261	-11.132		123.511	1.00 3		N
MOTA	1861	CA	GLY	Α	261	-11.138		122.631	1.00 4	4.49	С
ATOM	1862	С	GLY	Α	261	-9.848	53.579	121.840	1.00 4	2.98	С
ATOM	1863	0	GLY	Α	261	-8.758	53.595	122.411	1.00 5	1.16	0
MOTA	1864	N			262	-9.961	53.747		1.00 3		N
ATOM	1865	CA			262	-8.775		119.692	1.00 2		Ċ
ATOM	1866	c.			262	-8.810		118.761	1.00 1		č
MOTA	1867	ŏ			262	-9.877		118.407		6.05	ŏ
											ŏ
MOTA	1868	CB			262	-8.559		118.809	1.00 3		C
MOTA	1869	CG			262	-8.723		119.495	1.00 3		Ç
MOTA	1870		TRP			-9.808		119.450	1.00 3		C
MOTA	1871		TRP			-7.760		120.315	1.00 3		С
ATOM	1872		TRP		262	-9.582		120.192	1.00 3	7.75	N
ATOM	1873	CE2	TRP	Α	262	-8.330		120.737	1.00 4	3.01	С
MOTA	1874	CE3	TRP	Α	262	-6.471	51.101	120.742	1.00 4	6.70	С
MOTA	1875	CZ2	TRP	Α	262	-7.653		121.557	1.00 5	7.69	С
MOTA	1876		TRP		262	-5.796		121.562	1.00 5		С
ATOM	1877		TRP			-6.391		121.962	1.00 6		Ċ
ATOM	1878	N			263	-7.625		118.360	1.00 1		Ň
ATOM	1879	CA			263	-7.521					č
								117.409	1.00 1		Č
MOTA	1880	C			263	-7.642		116.036	1.00 1		c
ATOM	1881	0			263	-6.921		115.722	1.00 2		0
MOTA	1882	СВ	ASN			-6.182		117.545	1.00 2		С
MOTA	1883	CG	ASN	Α	263	-6.251	58.536	118.460	1.00 2	1.75	С
MOTA	1884	OD1	ASN	Α	263	-7.115	59.401	118.317	1.00 2	0.11	0
ATOM	1885	ND2	ASN	Α	263	-5.332	58.595	119.399	1.00 1	6.20	N
ATOM	1886	N	ASP	Α	264	-8.555	56.518	115.222	1.00	8.32	N
MOTA	1887	CA	ASP			-8.798		113.901	1.00 1		C
ATOM	1888	Ċ	ASP			-8.518		112.695	1.00 1		č
ATOM	1889	ŏ	ASP			-9.276		112.412		3.31	ŏ
ATOM	1890	СВ	ASP			-10.237		113.881	1.00 2		č
ATOM	1891										č
		CG	ASP			-10.832		112.491	1.00 2		
ATOM	1892		ASP			-10.208		111.574	1.00 1		0
ATOM	1893		ASP			-11.957		112.336	1.00 4		0
MOTA	1894	N	PRO			-7.413		111.965	1.00 1		N
MOTA	1895	CA	PRO	Α	265	-6.863	57.251	110.771	1.00 2	3.99	С
MOTA	1896	С	PRO	Α	265	-7.803	57.195	109.577	1.00 2	8.89	С
MOTA	1897	0	PRO	Α	265	-8.107	58.216	108.945	1.00 3	5.15	0
ATOM	1898	CB	PRO			-5.579	56.467	110.495	1.00 1	7.45	С
MOTA	1899	CG	PRO			-5.192		111.859	1.00 2		Č
ATOM	1900	CD	PRO			-6.517		112.391	1.00 1		Č
ATOM	1901	N	ASP			-8.207		109.272	1.00 3		Ň
	1902	CA	ASP			-9.136		108.202		1.09	č
MOTA											Č
ATOM	1903	C	ASP			-8.830		107.598	1.00 3		C
ATOM	1904	0	ASP			-7.910		108.015		6.66	0
MOTA	1905	CB	ASP			-9.162		107.092	1.00 4		C
MOTA	1906	CG	ASP			-10.562		106.559	1.00 4		С
ATOM	1907		ASP			-11.405		106.792	1.00 4	8.02	0
ATOM	1908	OD2	ASP	Α	266	-10.830	57.927	105.920	1.00 4	6.64	0
ATOM	1909	N	MET	Α	267	-9.619	53.896	106.604	1.00 3	6.60	N
ATOM	1910	CA	MET	Α	267	-9.475	52.620	105.944	1.00 3	4.79	С
ATOM	1911	Ċ	MET	Α	267	-8.076	52.362	105.395	1.00 2		С
ATOM	1912	ō	MET			-7.257		105.275	1.00 1		Ō
ATOM	1913	СВ	MET			-10.510		104.828	1.00 3		č
MOTA	1914	CG	MET			-11.920		105.337	1.00 3		Č
ATOM	1915	SD	MET			-13.059		104.118	1.00 5		š
								104.314			č
MOTA	1916	CE	MET			-12.830			1.00 6		N
MOTA	1917	N	LEU			-7.816		105.103	1.00 2		
ATOM	1918	CA	LEU			-6.560		104.530	1.00 2		С С О
MOTA	1919	C	LEU			-6.809		103.027	1.00 2		Ü
ATOM	1920	0	LEU			-7.592		102.572	1.00 3		
MOTA	1921	CB	LEU			-6.169		105.097	1.00 1		c c
MOTA	1922	CG	LEU			-5.596		106.516	1.00 2		С
MOTA	1923		LEU			-5.216		106.948	1.00 2		С
	1924	CD2	LEU	A	268	-4.380		106.550	1.00 2		Č
	1925	N	VAL			-6.151	51.390	102.256	1.00 2	7.46	N
	1926	CA	VAL			-6.334	51.398	100.813	1.00 3		С
MOTA	1927	C	VAL			-5.350		100.097	1.00 3		С
ATOM	1928	ō	VAL			-5.174	50.597	98.880	1.00 4		ō
	1929	ČВ	VAL			-6.190		100.274	1.00 3		Č
	1930		VAL			-7.094		101.067	1.00 4		č
ATOM	1931		VAL			-4.737		100.379	1.00 4		č
ATOM	1932	N	ILE			-4.702		100.864	1.00 2		N
	1933	CA	ILE			-3.735		100.309	1.00 2		č
ATOM							47.621	99.458			ċ
	1934	C	ILE			-4.487			1.00 3		
MOTA	1935	0	ILE	Α	2/0	-5.477	47.038	99.916	1.00 3	1.67	0

3 most	1016	^ D	***		270					_
MOTA	1936	СB		A	270	-2.956	47.944	101.446	1.00 27.69	С
MOTA	1937	CG1	ILE	A	270	-2.044	48.936	102.162	1.00 43.55	С
MOTA	1938	CG2	ILE	A	270	-2.106		100.888	1.00 29.54	č
	1939				270					
MOTA						-1.483	48.423		1.00 41.14	С
MOTA	1940	N	GLY	Α	271	-4.026	47.387	98.231	1.00 37.10	N
MOTA	1941	CA	GLY	Α	271	-4.697	46.416	97.381	1.00 42.05	С
MOTA	1942	С	GLY	A	271	-5.414	47.078		1.00 45.94	Ċ
ATOM	1943	ŏ			271	-5.978				
							46.417		1.00 46.95	0
MOTA	1944	N			272	-5.395	48.405		1.00 49.29	N
MOTA	1945	CA	ASN	Α	272	-6.013	49.196	95.189	1.00 50.77	С
MOTA	1946	С	ASN	Α	272	-4.955	49.544		1.00 54.19	C
ATOM	1947	ŏ			272	-4.165	48.688		1.00 62.17	ŏ
										ū
MOTA	1948	CB			272	-6.616	50.463		1.00 57.02	С
MOTA	1949	CG			272	-7.937	50.208	96.456	1.00 64.75	С
ATOM	1950	OD1	ASN	Α	272	-8.078	49.269	97.245	1.00 70.55	0
MOTA	1951	ND2	ASN	Α	272	-8.920	51.048		1.00 65.78	N
ATOM	1952	N			273	-4.906	50.803		1.00 57.71	
					273					N
ATOM	1953	CA				-3.961	51.221		1.00 60.84	С
MOTA	1954	С	PHE	Α	273	-3.119	52.455	92.989	1.00 59.50	С
MOTA	1955	0	PHE	Α	273	-2.030	52.593	92.439	1.00 61.91	0
MOTA	1956	CB	PHE	Α	273	-4.712	51.464	91.391	1.00 60.01	č
	1957	CG								
MOTA					273	-6.185	51.147		1.00 59.22	Č
MOTA	1958		PHE			-6.766	50.281	90.534	1.00 54.75	Ċ
MOTA	1959	CD2	PHE	Α	273	-6.985	51.679	92.475	1.00 58.02	Ċ
MOTA	1960	CE1	PHE	Α	273	-8.124	49.943		1.00 51.25	С
ATOM	1961		PHE			-8.336	51.354		1.00 58.47	č
										Č
MOTA	1962	CZ			273	-8.909	50.481		1.00 55.69	С
MOTA	1963	N	GLY	Α	274	-3.624	53.348	93.836	1.00 55.05	N
MOTA	1964	CA	GLY	Α	274	-2.914	54.580	94.139	1.00 44.40	С
ATOM	1965	C			274	-1.577	54.444		1.00 39.16	č
	1966	ŏ								
ATOM					274	-0.753	55.362		1.00 47.25	0
MOTA	1967	N			275	-1.344	53.307	95.475	1.00 28.25	N
MOTA	1968	CA	LEU	Α	275	-0.091	53.116	96.183	1.00 27.58	С
MOTA	1969	С	LEU	Α	275	0.928	52.199	95.542	1.00 32.09	С
ATOM	1970	ō			275	0.601	51.154	94.977	1.00 42.20	ŏ
ATOM	1971									
		CB			275	-0.360	52.640		1.00 16.36	Č
MOTA	1972	CG			275	-1.250	53.577	98.419	1.00 5.93	С
ATOM	1973	CD1	LEU	Α	275	-1.093	53.240	99.888	1.00 3.31	Ċ
MOTA	1974	CD2	LEU	А	275	-0.864	55.035	98.151	1.00 3.31	Ċ
ATOM	1975	N			276	2.180				
							52.628		1.00 29.50	N
MOTA	1976	CA			276	3.314	51.881	95.136	1.00 36.25	C
ATOM	1977	С	SER	Α	276	3.451	50.735	96.104	1.00 35.37	С
MOTA	1978	0	SER	Α	276	2.738	50.677	97.100	1.00 27.12	0
ATOM	1979	ĊВ			276	4.594	52.712	95.219	1.00 46.24	č
ATOM	1980	OG			276	5.122	52.704	96.541	1.00 42.54	0
MOTA	1981	N	TRP	A	277	4.371	49.826	95.833	1.00 37.28	N
ATOM	1982	CA	TRP	Α	277	4.540	48.740	96.762	1.00 32.97	С
MOTA	1983	C			277	5.008	49.364	98.048	1.00 27.84	Č
ATOM	1984	ŏ	TRP			4.267	49.420	99.028		
									1.00 25.18	0
MOTA	1985	CB	TRP			5.586	47.736	96.292	1.00 44.35	С
ATOM	1986	CG	TRP	Α	277	5.823	46.671	97.324	1.00 45.64	С
MOTA	1987	CD1	TRP	Α	277	7.004	46.389	97.961	1.00 49.91	С
MOTA	1988		TRP			4.839	45.797	97.898	1.00 45.05	Ċ
MOTA	1989	NE1	TRP			6.815	45.398	98.898	1.00 47.99	
										N
ATOM	1990		TRP			5.496	45.016	98.884	1.00 44.93	000
ATOM	1991	CE3	TRP	Α	277	3.465	45.599	97.680	1.00 43.84	С
ATOM	1992	CZ2	TRP	Α	277	4.820	44.047	99.657	1.00 41.10	С
MOTA	1993		TRP			2.793	44.637	98.447	1.00 38.42	Ċ
MOTA	1994		TRP			3.474	43.875	99.424	1.00 38.38	č
ATOM	1995	N	ASN			6.237	49.862	98.042	1.00 27.92	N
MOTA	1996	CA	ASN	Α	278	6.792	50.454	99.252	1.00 33.66	С
ATOM	1997	C	ASN	Α	278	5.887	51.473	99.939	1.00 36.34	С
MOTA	1998	Õ	ASN			6.108		101.096	1.00 40.73	ō
MOTA	1999					8.169	51.051		1.00 29.87	č
		СВ	ASN					98.967		Ľ.
MOTA	2000	CG	ASN			9.234	49.986	98.822	1.00 31.51	С
MOTA	2001	OD1	ASN	А	278	9.542	49.270	99.778	1.00 31.53	0
MOTA	2002	ND2	ASN	Α	278	9.791	49.862	97.618	1.00 36.12	N
MOTA	2003	N	GLN			4.869	51.957	99.238	1.00 35.96	N
ATOM	2004	CA	GLN			3.945	52.880			
								99.868	1.00 29.77	c
ATOM	2005	Ç	GLN			2.915		100.678	1.00 26.47	С
MOTA	2006	0	GLN	A	279	2.468		101.732	1.00 16.00	0
MOTA	2007	CB	GLN	Α	279	3.267	53.743	98.810	1.00 27.43	С
MOTA	2008	CG	GLN			4.137	54.893	98.349	1.00 28.81	č
MOTA										ž
	2009	CD	GLN			3.737	55.417	96.991	1.00 34.90	c
MOTA	2010		GLN			2.550	55.562	96.694	1.00 40.75	0
MOTA	2011	NE2	GLN	Α	279	4.727	55.712	96.155	1.00 39.37	N
MOTA	2012	N	GLN			2.567	50.897	100.196	1.00 30.38	N
MOTA	2013	CA	GLN			1.595		100.881	1.00 30.96	Ċ
ATOM	2014							102.189		Ċ
		C	GLN			2.139			1.00 30.35	
MOTA	2015	0	GLN			1.480		103.228	1.00 33.06	Ō
MOTA	2016	CB	GLN	A	280	1.164	48.895	99.999	1.00 31.33	С

MOTA	2017	CG				1.00 36.80	С
MOTA	2018	CD				1.00 37.60	Ç
MOTA	2019		1 GLN A 280			1.00 38.74	0
ATOM	2020		2 GLN A 280			1.00 34.63	N
ATOM	2021 2022	N CA	VAL A 281 VAL A 281			1.00 31.13	N
MOTA MOTA	2022	C	VAL A 281			1.00 35.92 1.00 33.94	C C
MOTA	2024	ŏ	VAL A 281			1.00 33.34	0
ATOM	2025	СВ				1.00 31.74	c
ATOM	2026		1 VAL A 281			1.00 34.63	č
ATOM	2027		2 VAL A 281			1.00 42.38	č
MOTA	2028	N	THR A 282			1.00 31.90	Ň
MOTA	2029	CA	THR A 282	4.186		1.00 27.13	Ċ
ATOM	2030	С	THR A 282	2.872		1.00 26.03	Ċ
ATOM	2031	0	THR A 282			1.00 28.72	0
MOTA	2032	CB	THR A 282			1.00 26.85	С
MOTA	2033		1 THR A 282			1.00 31.54	Ō
MOTA MOTA	2034 2035		2 THR A 282 GLN A 283			1.00 20.56	C.
ATOM	2036	N CA	GLN A 283			1.00 18.46	N
ATOM	2037	C	GLN A 283			1.00 18.53 1.00 18.82	C C
ATOM	2038	ŏ	GLN A 283			1.00 21.00	Ö
ATOM	2039	СB	GLN A 283			1.00 15.63	č
ATOM	2040	CG	GLN A 283			1.00 19.59	č
MOTA	2041	CD	GLN A 283	-3.291	52.386 104.495	1.00 27.53	C
MOTA	2042		L GLN A 283			1.00 31.55	0
MOTA	2043		2 GLN A 283			1.00 35.44	N
ATOM	2044	N	MET A 284			1.00 3.31	N
MOTA	2045	CA	MET A 284			1.00 3.31	С
ATOM ATOM	2046 2047	C	MET A 284			1.00 3.31	c
ATOM	2047	CB	MET A 284 MET A 284			1.00 7.85	0
ATOM	2049	CG	MET A 284			1.00 8.74 1.00 6.90	c c
ATOM	2050	SD	MET A 284			1.00 16.54	s
ATOM	2051	CE	MET A 284		46.136 108.956	1.00 6.72	č
ATOM	2052	N	ALA A 285			1.00 4.64	N
MOTA	2053	CA	ALA A 285	3.375	49.193 109.041	1.00 11.01	Ċ
MOTA	2054	С	ALA A 285		50.228 110.059	1.00 13.01	С
ATOM	2055	0	ALA A 285			1.00 14.68	0
ATOM	2056	CB	ALA A 285		49.530 108.521	1.00 19.24	С
ATOM	2057	N	LEU A 286		51.419 109.585	1.00 11.37	N
MOTA MOTA	2058 2059	CA	LEU A 286 LEU A 286			1.00 14.05	C
ATOM	2060	ò	LEU A 286		52.342 111.166 52.755 112.321	1.00 17.26	C
ATOM	2061	ČВ	LEU A 286		53.826 109.826	1.00 15.35 1.00 8'.12	0 C
ATOM	2062	ĊĞ	LEU A 286		54.187 109.997	1.00 7.08	Ċ
ATOM	2063		LEU A 286		54.888 108.795	1.00 9.40	č
ATOM	2064	CD2	LEU A 286	4.116	55.041 111.246	1.00 3.31	Ċ
ATOM	2065	N	TRP A 287	-0.119	51.774 110.491	1.00 17.25	N
MOTA	2066	CA	TRP A 287	-1.405	51.613 111.168	1.00 29.47	С
ATOM	2067	C	TRP A 287	-1.166	50.692 112.360	1.00 31.64	C
ATOM ATOM	2068 2069	O CB	TRP A 287	-1.783	50.850 113.419	1.00 33.74	0
ATOM	2070	CG	TRP A 287	-2.459 -3.358	50.998 110.256 52.007 109.618	1.00 33.70 1.00 39.21	C C
ATOM	2071		TRP A 287	-4.717	51.949 109.526	1.00 47.57	c
ATOM	2072		TRP A 287	-2.966	53.217 108.969	1.00 36.94	Ċ
ATOM	2073		TRP A 287	-5.197	53.046 108.861	1.00 51.26	N
ATOM	2074	CE2	TRP A 287	-4.144	53.841 108.509	1.00 40.64	Ċ
ATOM	2075		TRP A 287		53.834 108.730	1.00 39.12	С
MOTA	2076		TRP A 287	-4.126	55.056 107.823	1.00 40.95	С
MOTA	2077		TRP A 287	-1.715	55.047 108.043	1.00 37.09	Ċ
MOTA	2078		TRP A 287	-2.908	55.643 107.599	1.00 35.17	C
ATOM ATOM	2079 2080	N CA	ALA A 288 ALA A 288	-0.257 0.097	49.740 112.178 48.809 113.235	1.00 26.74	N
ATOM	2081	c	ALA A 288	0.749	49.570 114.388	1.00 26.87 1.00 29.10	C C
ATOM	2082	ŏ	ALA A 288	0.472	49.296 115.560	1.00 29.10	ò
MOTA	2083	ČВ	ALA A 288	1.048	47.755 112.706	1.00 25.97	č
MOTA	2084	N	ILE A 289	1.616	50.525 114.059	1.00 26.15	N
ATOM	2085	CA	ILE A 289	2.290	51.310 115.089	1.00 21.64	С
ATOM	2086	Ċ	ILE A 289	1.299	52.166 115.840	1.00 21.16	C
ATOM	2087	O CB	ILE A 289	1.436	52.349 117.045	1.00 18.99	0
MOTA MOTA	2088 2089	CB CG1	ILE A 289 ILE A 289	3.339	52.254 114.507	1.00 20.59	C C
ATOM	2090		ILE A 289	4.512 3.808	51.441 113.947 53.233 115.593	1.00 17.18 1.00 29.08	Ċ
MOTA	2091		ILE A 289	5.332	50.768 115.030	1.00 23.00	c
MOTA	2092	N	MET A 290	0.299	52.683 115.128	1.00 23.88	N
MOTA	2093 -	CA	MET A 290	-0.715	53.550 115.734	1.00 30.50	С
MOTA	2094	C	MET A 290	-1.986	52.847 116.198	1.00 30.09	С
ATOM	2095	0	MET A 290	-3.072	53.425 116.084	1.00 35.20	0
ATOM ATOM	2096 2097	CB CG	MET A 290 MET A 290	-1.134	54.643 114.755 55.363 114.077	1.00 32.03	c
011	20,		A 230	-0.012	33.303 114.077	1.00 39.82	С

MOTA	2098	SD	MET A 290	-0.757	56.559 113.005	1.00 26.07	:
MOTA	2099	CE	MET A 290	-1.038	55.555 111.564	1.00 23.83	
MOTA	2100	N	ALA A 291	-1.858	51.631 116.725	1.00 30.09	1
MOTA	2101	CA	ALA A 291	-3.019	50.884 117.187	1.00 31.39	
MOTA	2102	C	ALA A 291	-4.246	51.539 116.582	1.00 32.14	
MOTA MOTA MOTA	2103 2104 2105	O CB N	ALA A 291 ALA A 291 ALA A 292	-5.031 -3.096 -4.367	52.191 117.271 50.916 118.700 51.410 115.269	1.00 25.20 1.00 34.14 1.00 33.73	((
MOTA	2106	CA	ALA A 292	-5.487	51.998 114.554	1.00 36.12	(
MOTA	2107	C	ALA A 292	-6.433	50.912 114.096	1.00 30.80	
ATOM ATOM ATOM	2108 2109 2110	O CB N	ALA A 292 ALA A 292 PRO A 293	-6.022 -4.986 -7.720	49.769 113.869 52.785 113.346 51.250 113.951	1.00 32.69 1.00 46.22 1.00 28.94	((
MOTA	2111	CA	PRO A 293	-8.632	50.202 113.506	1.00 24.30	(
MOTA	2112	C	PRO A 293	-8.208	49.776 112.092	1.00 15.99	
MOTA	2113	O	PRO A 293	-7.829	50.617 111.265	1.00 15.74	(
MOTA	2114	CB	PRO A 293	-9.994	50.899 113.527	1.00 26.38	
MOTA	2115	CG	PRO A 293	-9.814	52.021 114.504	1.00 34.28	
MOTA MOTA MOTA	2116 2117 2118	CD N CA	PRO A 293 LEU A 294 LEU A 294	-8.436 -8.262 -7.890	52.516 114.177 48.475 111.824 47.958 110.510	1.00 29.52 1.00 19.73 1.00 26.53	(!
MOTA	2119	С	LEU A 294	-9.101	47.695 109.638	1.00 22.11	(
MOTA	2120	0	LEU A 294	-9.781	46.675 109.795	1.00 22.16	
ATOM	2121	CB	LEU A 294	-7.091	46.666 110.654	1.00 33.64	(
ATOM	2122	CG	LEU A 294	-5.896	46.869 111.584	1.00 32.51	
ATOM	2123	CD1	LEU A 294	-5.175	45.550 111.775	1.00 39.27	
MOTA MOTA MOTA	2124 2125 2126	CD2 N CA	LEU A 294 PHE A 295 PHE A 295	-4.966 -9.380 -10.496	47.929 111.011 48.626 108.734 48.461 107.826	1.00 38.99 1.00 15.76 1.00 22.79	; ;
MOTA	2127	С	PHE A 295	-10.057	48.611 106.398	1.00 21.95	(
MOTA	2128	0	PHE A 295	-9.621	49.684 105.978	1.00 33.01	
ATOM	2129	CB	PHE A 295	-11.591	49.461 108.128	1.00 34.79	(
ATOM	2130	CG	PHE A 295	-12.427	49.066 109.284	1.00 37.92	
ATOM	2131	CD1	PHE A 295	-11.858	48.912 110.538	1.00 41.65	
ATOM ATOM ATOM	2132 2133 2134	CE1	PHE A 295 PHE A 295 PHE A 295	-13.779 -12.623 -14.557	48.796 109.120 48.488 111.617 48.373 110.192	1.00 38.93 1.00 41.88 1.00 43.07	(
MOTA	2135	CZ	PHE A 295	-13.976	48.219 111.446	1.00 41.57	1
MOTA	2136	N	MET A 296	-10.157	47.526 105.647	1.00 16.43	
MOTA	2137	CA	MET A 296	-9.772	47.568 104.264	1.00 20.20	(
ATOM	2138	C	MET A 296	-10.900	48.240 103.506	1.00 24.39	
ATOM	2139	O	MET A 296	-12.021	48.359 104.008	1.00 27.05	
ATOM	2140	CB	MET A 296	-9.584	46.158 103.740	1.00 19.92	(
ATOM	2141	CG	MET A 296	-8.577	45.336 104.497	1.00 34.51	
ATOM	2142	SD	MET A 296	-8.572	43.657 103.898	1.00 39.83	
ATOM	2143	CE	MET A 296	-9.951	42.993 104.798	1.00 45.94	1
ATOM	2144	N	SER A 297	-10.578	48.703 102.308	1.00 27.42	
ATOM	2145	CA	SER A 297	-11.539	49.327 101.435	1.00 25.61	
MOTA	2146	C	SER A 297	-10.968	48.931 100.097	1.00 25.82	(
MOTA	2147	O	SER A 297	-10.318	49.718 99.404	1.00 20.60	
ATOM	2148	CB	SER A 297	-11.530	50.840 101.585	1.00 34.64	(
ATOM	2149	OG	SER A 297	-12.538	51.408 100.771	1.00 33.54	
ATOM	2150	N	ASN A 298	-11.179	47.673 99.753	1.00 31.94	
ATOM	2151	CA	ASN A 298	-10.675	47.144 98.504	1.00 37.75	(
ATOM	2152	C	ASN A 298	-11.640	46.084 98.022	1.00 39.05	
ATOM	2153	O	ASN A 298	-12.508	45.647 98.771	1.00 40.73	
MOTA	2154	CB	ASN A 298	-9.292	46.534 98.730	1.00 41.55	(
MOTA	2155	CG	ASN A 298	-9.217	45.733 100.025	1.00 41.53	
ATOM ATOM ATOM	2156 2157 2158	ND2 N	ASN A 298 ASN A 298 ASP A 299	-9.945 -8.343 -11.506	44.764 100.207 46.148 100.934 45.687 96.765	1.00 44.50 1.00 41.54 1.00 36.81) 1 1
MOTA MOTA MOTA	2159 2160 2161	CA C	ASP A 299 ASP A 299 ASP A 299	-12.358 -11.584 -10.636	44.650 96.223 43.354 96.440 43.074 95.710	1.00 37.64 1.00 35.85 1.00 33.62	(
MOTA MOTA MOTA	2162 2163 2164	CB CG	ASP A 299 ASP A 299 ASP A 299	-12.583 -13.527 -13.591	44.871 94.736 43.859 94.144 42.740 94.685	1.00 43.70 1.00 54.79 1.00 67.53	(
MOTA	2165	OD2	ASP A 299	-14.190	44.167 93.132	1.00 67.01	
MOTA	2166	N	LEU A 300	-11.976	42.584 97.455	1.00 32.08	
MOTA	2167	CA	LEU A 300	-11.327	41.310 97.790	1.00 30.22	(
MOTA	2168	C	LEU A 300	-11.470	40.241 96.684	1.00 35.38	
MOTA	2169	O	LEU A 300	-10.860	39.162 96.753	1.00 42.36	
ATOM	2170	CB	LEU A 300	-11.907	40.743 99.096	1.00 18.15	(
ATOM	2171	CG	LEU A 300	-11.796	41.541 100.401	1.00 30.55	
ATOM	2172	CD1	LEU A 300	-12.475	42.884 100.243	1.00 29.26	
MOTA	2173	CD2	LEU A 300	-12.442	40.763 101.546	1.00 33.51	(
MOTA	2174	N	ARG A 301	-12.298	40.519 95.680	1.00 37.98	!
MOTA MOTA MOTA	2175 2176 2177	CA C	ARG A 301 ARG A 301 ARG A 301	-12.507 -11.295 -10.744	39.574 94.583 39.662 93.686 38.653 93.259	1.00 42.73 1.00 53.30 1.00 57.15	(
MOTA	2178	СВ	ARG A 301	-13.769	39.944 93.799	1.00 34.40	(

ATOM	2179	CG	ARG	Α	301	-14.984	40.079	94.705	1 00	24.85	С
ATOM	2180	CD	ARG			-16.235					č
	2181						40.592	94.000		25.32	N
MOTA		NE			301	-16.077	41.935	93.443		41.71	
ATOM	2182	CZ	ARG			-17.092	42.734	93.121		44.10	C
ATOM	2183		ARG			-18.343	.42.330	93.308		50.21	N
MOTA	2184		ARG			-16.855	43.927	92.591		42.60	N
MOTA	2185	N	HIS			-10.878	40.889	93.415		63.36	N
MOTA	2186	CA	HIS			-9.731	41.118	92.565		70.59	Ċ
MOTA	2187	С	HIS			-8.688	41.887	93.338	1.00	66.36	С
ATOM	2188	0	HIS			-8.665	43.112	93.328	1.00	73.44	0
MOTA	2189	CB	HIS	Α	302	-10.185	41.869	91.324	1.00	77.08	С
MOTA	2190	CG	HIS	Α	302	-11.304	41.185	90.607	1.00	87.66	С
MOTA	2191	ND1	HIS	Α	302	-11.985	41.760	89.558	1.00	94.33	N
MOTA	2192	CD2	HIS	Α	302	-11.867	39.968	90.799	1.00	93.17	С
MOTA	2193	CE1	HIS	Α	302	-12.920	40.929	89.136	1.00	95.03	С
ATOM	2194	NE2	HIS	Α	302	-12.869	39.834	89.873	1.00	96.98	N
MOTA	2195	N	ILE	Α	303	-7.826	41.137	94.013	1.00	53.55	N
MOTA	2196	CA	ILE	Α	303	-6.771	41.706	94.827	1.00	35.96	С
MOTA	2197	С	ILE			-5.493	40.928	94.609		34.98	С
MOTA	2198	0	ILE	Α	303	-5.501	39.701	94.600		29.95	0
MOTA	2199	CB	ILE			-7.135	41.631	96.316		27.37	С
ATOM	2200		ILE			-6.021	42.250	97.160		23.79	Ċ
ATOM	2201		ILE			-7.341	40.183	96.716	1.00	32.58	
ATOM	2202		ILE			-6.378	42.429	98.601		29.68	č
ATOM	2203	N	SER			-4.397	41.655	94.436		33.35	N
ATOM	2204	CA	SER			-3.086	41.056	94.218		29.72	ċ
ATOM	2205	c	SER			-2.734	40.021	95.283		24.66	č
MOTA	2206	ŏ	SER			-3.131	40.143	96.444		21.66	Ċ
MOTA	2207	СВ	SER			-2.024	42.159	94.191		37.18	č
MOTA	2208	OG	SER			-2.505	43.327	94.844		41.23	ŏ
ATOM	2209	N	PRO			-1.983	38.981	94.904		28.02	N
ATOM	2210	ÇA	PRO			-1.610	37.957	95.881		31.32	Č
ATOM	2211	Č	PRO			-0.597	38.587	96.792		35.76	č
		Ö	PRO			-0.626		97.999			o
MOTA	2212		PRO				38.392	95.025		33.70	
ATOM	2213	CB				-0.979	36.866		1.00	31.17	C
MOTA	2214	CG	PRO			-1.551	37.108	93.662		36.08	C
ATOM	2215	CD	PRO			-1.528	38.601	93.563	1.00	36.70	C
ATOM	2216	N	GLN			0.302	39.351	96.177		42.85	N
ATOM	2217	CA	GLN			1.357	40.046	96.899		57.20	C
ATOM	2218	C	GLN			0.745	40.974	97.942		57.39	C
ATOM	2219	0	GLN			1.282	41.138	99.040		57.53	0
ATOM	2220	CB	GLN			2.243	40.837	95.923		66.11	C
MOTA	2221	CG	GLN			1.492	41.722	94.945		85.74	C
ATOM	2222	CD	GLN			2.427	42.537	94.062		95.69	c
ATOM	2223	OE1	GLN			3.256	41.987	93.337	1.00	94.96	0
ATOM	2224	NE2	GLN			2.294	43.857	94.119		99.44	N
MOTA	2225	N	ALA			-0.395	41.566	97.605		57.94	N
MOTA	2226	CA	ALA			-1.076	42.463	98.524		51.17	C
ATOM	2227	C	ALA			-1.655	41.654	99.667		44.95	С
MOTA	2228	0	ALA			-1.232		100.805		39.07	0
MOTA	2229	CB	ALA			-2.179	43.202	97.809		55.61	C
ATOM	2230	N	LYS			-2.621	40.796	99.352		42.01	· N
ATOM	2231	CA	LYS			-3.268		100.350		47.04	С
ATOM	2232	С	LYS	Α	308	-2.281		101.354		50.29	С
MOTA	2233	0	LYS			-2.623		102.513		47.87	0
MOTA	2234	CB	LYS			-3.994	38.784	99.671		55.40	С
ATOM	2235	CG	LYS			-4.576		100.662		60.40	С
MOTA	2236	CD	LYS			-4.896	36.445	100.006		67.45	С
MOTA	2237	CE	LYS	Α	308	-3.630	35.772	99.525	1.00	70.11	С
MOTA	2238	NZ	LYS	Α	308	-3.911		99.008	1.00	71.25	N
MOTA	2239	N	ALA	Α	309	-1.064		100.890	1.00	51.68	N
ATOM	2240	CA	ALA	Α	309	-0.020	38.525	101.736	1.00	47.05	С
MOTA	2241	С	ALA	Α	309	0.271	39.497	102.860		41.92	С
ATOM	2242	0	ALA	Α	309	0.223	39.152	104.043	1.00	39.00	0
ATOM	2243	CB	ALA	Α	309	1.235	38.288	100.929	1.00	48.75	С
ATOM	2244	N	LEU	Α	310	0.575		102.473	1.00	38.55	N
MOTA	2245	CA	LEU	Α	310	0.862	41.776	103.431	1.00	35.05	C
MOTA	2246	С	LEU	A	310	-0.327		104.350		31.60	С
ATOM	2247	0	LEU			-0.208		105.546	1.00	36.47	0
MOTA	2248	CB	LEU			1.156		102.692	1.00	40.89	С
MOTA	2249	CG	LEU	Α	310	1.351		103.492		41.10	c
MOTA	2250	CD1	LEU	Α	310	2.416		104.544		53.29	С
MOTA	2251	CD2	LEU	Α	310	1.742		102.549		32.28	С
ATOM	2252	N	LEU	Α	311	-1.475		103.782		31.14	N
ATOM	2253	CA	LEU	Α	311	-2.695		104.554		33.68	С
MOTA	2254	C	LEU			-2.941		105.655		28.45	ç
MOTA	2255	0	LEU			-3.516		106.724		17.90	Ō
ATOM	2256	CB	LEU			-3.896		103.603		30.88	Ċ
ATOM	2257	CG	LEU			-4.044		102.895		37.10	Ċ
MOTA	2258		LEU			-4.744		101.566		32.41	Ç
MOTA	2259	CD2	LEU	Α	311	-4.805	44.869	103.803	1.00	41.72	С

ATOM	2260	N GLN A 312	2 404	40 363 105 405	1 00 27 61	.,
			-2.484	40.263 105.405	1.00 27.61	N
MOTA	2261	CA GLN A 312	-2.674	39.162 106.353	1.00 30.22	С
ATOM	2262	C GLN A 312	-1.445	38.737 107.173	1.00 35.43	Ċ
ATOM	2263					
		O GLN A 312	-1.537	37.806 107.965	1.00 35.04	0
ATOM	2264	CB GLN A 312	-3.223	37.936 105.610	1.00 25.27	C
MOTA	2265	CG GLN A 312	-4.519	38.187 104.853	1.00 29.16	Ċ
ATOM	2266	CD GLN A 312	-5.153	36.907 104.370	1.00 34.59	C
ATOM	2267	OE1 GLN A 312	-4.476	36.038 103.828	1.00 40.71	0
ATOM	2268	NE2 GLN A 312	-6.461	36.782 104.560		
					1.00 42.85	N
ATOM	2269	N ASP A 313	-0.309	39.406 106.999	1.00 42.55	N
MOTA	2270	CA ASP A 313	0.896	39.037 107.743	1.00 51.48	С
ATOM	2271	C ASP A 313				
			0.644	38.869 109.239	1.00 56.83	С
ATOM	2272	O ASP A 313	0.501	39.845 109.970	1.00 57.24	0
MOTA	2273	CB ASP A 313	2.004	40.071 107.535	1.00 56.92	Ċ
						_
MOTA	2274	CG ASP A 313	3.332	39.627 108.137	1.00 63.98	С
MOTA	2275	OD1 ASP A 313	3.327	39.138 109.292	1.00 75.54	0
MOTA	2276	OD2 ASP A 313	4.376	39.774 107.462	1.00 63.30	0
	2277					
MOTA		N LYS A 314	0.628	37.615 109.680	1.00 65.49	N
ATOM	2278	CA LYS A 314	0.374	37.256 111.078	1.00 66.96	C
ATOM	2279	C LYS A 314	1.141	38.065 112.103	1.00 57.67	Ċ
ATOM	2280	O LYS A 314	0.578	38.489 113.111	1.00 57.17	0
ATOM	2281	CB LYS A 314	0.675	35.772 111.310	1.00 82.41	С
MOTA	2282	CG LYS A 314	-0.131	34.821 110.436	1.00107.34	Č
						_
MOTA	2283	CD LYS A 314	0.257	33.378 110.710	1.00121.94	Č
ATOM	2284	CE LYS A 314	-0.587	32.410 109.897	1.00128.64	С
ATOM	2285	NZ LYS A 314	-0.280	30.993 110.247	1.00133.21	N
MOTA	2286	N ASP A 315	2.426	38.267 111.840	1.00 54.28	N
MOTA	2287	CA ASP A 315	3.304	39.000 112.751	1.00 54.88	C
ATOM	2288	C ASP A 315	3.004		1.00 53.15	č
				40.490 112.850		
MOTA	2289	O ASP A 315	3.227	41.108 113.891	1.00 57.46	0
ATOM	2290	CB ASP A 315	4.753	38.807 112.317	1.00 53.56	С
						~
MOTA	2291		5.064	37.365 111.983	1.00 53.59	С
ATOM	2292	OD1 ASP A 315	5.195	36.550 112.924	1.00 45.91	0
ATOM	2293	OD2 ASP A 315	5.162	37.051 110.775	1.00 56.89	0
	2294					
ATOM		N VAL A 316	2.513	41.072 111.764	1.00 44.71	N
ATOM	2295	CA VAL A 316	2.200	42.491 111.772	1.00 43.05	C
MOTA	2296	C VAL A 316	0.828	42.730 112.393	1.00 41.13	Ċ
ATOM	2297					ŏ
			0.645	43.676 113.168	1.00 48.44	U
ATOM	2298	CB VAL A 316	2.239	43.065 110.351	1.00 43.95	C
ATOM	2299	CG1 VAL A 316	1.943	44.552 110.380	1.00 47.89	С
MOTA	2300	CG2 VAL A 316	3.611			č
				42.817 109.740	1.00 47.49	
MOTA	2301	N ILE A 317	-0.132	41.871 112.059	1.00 34.07	N
ATOM	2302	CA ILE A 317	-1.468	41.999 112.618	1.00 30.90	С
MOTA	2303	C ILE A 317	-1.337	41.899 114.128		č
					1.00 38.79	C
ATOM	2304	O ILE A 317	-2.001	42.626 114.869	1.00 40.90	0
ATOM	2305	CB ILE A 317	-2.379	40.878 112.164	1.00 33.91	С
ATOM	2306	CG1 ILE A 317				č
			-2.279	40.715 110.657	1.00 45.06	C
MOTA	2307	CG2 ILE A 317	-3.797	41.187 112.572	1.00 24.03	Ċ
ATOM	2308	CD1 ILE A 317	-3.069	39.541 110.118	1.00 58.36	C
ATOM	2309	N ALA A 318	-0.475	40.981 114.564	1.00 43.73	N
						14
ATOM	2310	CA ALA A 318	-0.211	40.746 115.978	1.00 45.24	С
MOTA	2311	C ALA A 318	0.210	42.043 116.640	1.00 41.00	С
ATOM	2312	O ALA A 318	-0.322	42.423 117.681	1.00 47.27	ō
						· ·
ATOM	2313	CB ALA A 318	0.880	39.711 116.139	1.00 50.89	С
ATOM	2314	N ILE A 319	1.177	42.726 116.046	1.00 35.38	N
ATOM	2315	CA ILE A 319	1.617	43.989 116.611	1.00 37.59	С
ATOM	2316					
		C ILE A 319	0.436	44.946 116.776	1.00 42.37	C
MOTA	2317	O ILE A 319	0.174	45.410 117.886	1.00 51.31	0
ATOM	2318	CB ILE A 319	2.701	44.630 115.736	1.00 33.50	С
ATOM	2319	CG1 ILE A 319	4.004	43.851 115.906	1.00 36.32	č
MOTA	2320	CG2 ILE A 319	2.907	46.080 116.121	1.00 24.15	С
ATOM	2321	CD1 ILE A 319	5.096	44.312 115.001	1.00 50.54	C
ATOM	2322	N ASN A 320	-0.279	45.226 115.687	1.00 41.39	N
						- 14
ATOM	2323	CA ASN A 320	-1.430	46.118 115.752	1.00 44.04	c c
ATOM	2324	C ASN A 320	-2.487	45.624 116.751	1.00 42.92	c
ATOM	2325	O ASN A 320	-3.166	46.432 117.402	1.00 42.62	ŏ
						ž
ATOM	2326	CB ASN A 320	-2.052	46.264 114.360	1.00 48.77	C
ATOM	2327	CG ASN A 320	-3.400	46.972 114.389	1.00 49.02	С
MOTA	2328	OD1 ASN A 320	-4.366	46.460 114.947	1.00 50.55	Ō
ATOM	2329	ND2 ASN A 320		48.153 113.781		
			-3.468		1.00 48.27	N
MOTA	2330	N GLN A 321	-2.614	44.300 116.865	1.00 41.27	N
MOTA	2331	CA GLN A 321	-3.575	43.655 117.770	1.00 42.11	С
ATOM	2332	C GLN A 321	-3.035	43.442 119.185	1.00 37.90	Č
ATOM	2333	O GLN A 321	-3.636	42.716 119.991	1.00 38.05	0
ATOM	2334	CB GLN A 321	-3.999	42.297 117.213	1.00 47.40	Ċ
ATOM	2335	CG GLN A 321		42.376 116.132		ž
			-5.033		1.00 44.04	C
ATOM	2336	CD GLN A 321	-6.282	43.051 116.621	1.00 38.41	С
MOTA	2337	OE1 GLN A 321	-6.794	42.726 117.686	1.00 20.43	0
ATOM	2338	NE2 GLN A 321	-6.785	43.995 115.843	1.00 37.61	N
MOTA	2339	N ASP A 322	-1.898	44.067 119.479	1.00 34.86	N
MOTA	2340	CA ASP A 322	-1.281	43.948 120.794	1.00 33.53	С
						=

ATOM	2341 C ASP A 322	-2.363 44.148 121.849 1.00 29.16	С
MOTA	2342 O ASP A 322	-3.154 45.089 121.773 1.00 29.97	0
MOTA	2343 CB ASP A 322	-0.175 44.993 120.944 1.00 40.79	С
ATOM	2344 CG ASP A 322	0.655 44.782 122.180 1.00 43.03	С
ATOM	2345 OD1 ASP A 322	1.207 43.675 122.350 1.00 32.44	0
ATOM	2346 OD2 ASP A 322	0.757 45.735 122.972 1.00 51.49	Ó
ATOM	2347 N PRO A 323	-2.405 43.258 122.846 1.00 26.74	N
MOTA	2348 CA PRO A 323	-3.383 43.290 123.935 1.00 31.97	Ċ
MOTA	2349 C PRO A 323	~3.221 44.500 124.811 1.00 35.44	Ċ
MOTA	2350 O PRO A 323	-4.189 45.007 125.369 1.00 43.01	ō
ATOM	2351 CB PRO A 323	-3.083 42.010 124.691 1.00 39.61	č
ATOM	2352 CG PRO A 323	-1.584 41.978 124.624 1.00 39.47	č
ATOM	2353 CD PRO A 323	-1.309 42.325 123.163 1.00 35.67	. ç
ATOM	2354 N LEU A 324	-1.979 44.947 124.925 1.00 36.88	N
ATOM	2355 CA LEU A 324	-1.653 46.084 125.758 1.00 40.93	ċ
ATOM	2356 C LEU A 324	-2.498 47.299 125.407 1.00 40.56	č
ATOM	2357 O LEU A 324	-3.158 47.872 126.275 1.00 45.00	ŏ
MOTA	2358 CB LEU A 324	-0.169 46.427 125.628 1.00 46.67	č
ATOM	2359 CG LEU A 324	0.519 46.892 126.915 1.00 54.17	č
ATOM	2360 CD1 LEU A 324	1.848 47.528 126.556 1.00 62.38	Č
ATOM	2361 CD2 LEU A 324	-0.355 47.894 127.656 1.00 53.61	ç
ATOM	2362 N GLY A 325	-2.463 47.699 124.139 1.00 38.97	N
ATOM	2363 CA GLY A 325	-3.242 48.846 123.708 1.00 41.98	C
ATOM	2364 C GLY A 325	-2.527 50.166 123.912 1.00 47.29	Č
ATOM	2365 O GLY A 325	-3.148 51.170 124.264 1.00 52.51	
ATOM	2366 N LYS A 326	-1.217 50.163 123.696 1.00 48.67	0
ATOM	2367 CA LYS A 326	-0.414 51.368 123.850 1.00 49.67	N
ATOM	2368 C LYS A 326		C
ATOM	2369 O LYS A 326		C
MOTA			0
ATOM	2370 CB LYS A 326 2371 CG LYS A 326	0.862 51.038 124.622 1.00 56.04 0.628 50.710 126.086 1.00 73.85	C
ATOM			C
ATOM		0.246 51.950 126.890 1.00 82.94 1.430 52.903 127.054 1.00 88.67	C
MOTA	2373 CE LYS A 326 2374 NZ LYS A 326		Ç
ATOM	2374 NZ LIS A 326 2375 N GLN A 327		N
ATOM		-0.724 52.998 122.071 1.00 48.25	N
ATOM		-0.491 53.573 120.746 1.00 50.19	C
ATOM		0.920 54.090 120.541 1.00 45.92	C
MOTA		1.492 54.715 121.423 1.00 47.59	0
		-1.504 54.687 120.457 1.00 46.44	C
ATOM	2380 CG GLN A 327	-1.652 55.028 118.977 1.00 36.98	Ç
MOTA	2381 CD GLN A 327	-3.034 55.579 118.640 1.00 41.12	C
MOTA	2382 OE1 GLN A 327	-4.041 54.862 118.680 1.00 47.47	0
ATOM	2383 NE2 GLN A 327	-3.085 56.858 118.309 1.00 34.38	N
MOTA	2384 N GLY A 328	1.470 53.820 119.361 1.00 36.61	N
ATOM	2385 CA GLY A 328	2.818 54.249 119.043 1.00 29.84	C
MOTA	2386 C GLY A 328	2.895 55.741 118.822 1.00 27.35	Ç
ATOM	2387 O GLY A 328	1.923 56.463 119.057 1.00 29.82	0
ATOM	2388 N TYR A 329	4.050 56.202 118.358 1.00 29.39	N
MOTA	2389 CA TYR A 329	4.268 57.622 118.118 1.00 35.23	С
MOTA	2390 C TYR A 329	5.595 57.878 117.421 1.00 37.00	С
ATOM	2391 O TYR A 329	6.515 57.060 117.470 1.00 36.29	0
ATOM	2392 CB TYR A 329	4.276 58.369 119.443 1.00 38.53	С
MOTA	2393 CG TYR A 329	5.275 57.798 120.422 1.00 46.66	С
ATOM	2394 CD1 TYR A 329	6.643 57.993 120.250 1.00 48.72	С
MOTA	2395 CD2 TYR A 329	4.850 57.025 121.508 1.00 51.95	С
ATOM	2396 CE1 TYR A 329	7.562 57.430 121.136 1.00 49.58	С
MOTA	2397 CE2 TYR A 329	5.759 56.461 122.397 1.00 51.04	С
ATOM	2398 CZ TYR A 329	7.111 56.665 122.207 1.00 46.71	C
ATOM	2399 OH TYR A 329	8.015 56.100 123.078 1.00 44.19	0
ATOM	2400 N GLN A 330	5.693 59.036 116.787 1.00 37.71	N
MOTA	2401 CA GLN A 330	6.915 59.419 116.108 1.00 32.77	С
ATOM	2402 C GLN A 330	7.949 59.763 117.168 1.00 34.91	С
MOTA	2403 O GLN A 330	7.664 60.480 118.118 1.00 29.29	0
MOTA	2404 CB GLN A 330	6.661 60.636 115.228 1.00 29.38	c c
MOTA	2405 CG GLN A 330	7.876 61.132 114.480 1.00 37.88	С
ATOM	2406 CD GLN A 330	7.614 62.464 113.828 1.00 50.08	C
ATOM	2407 OE1 GLN A 330	7.393 63.461 114.508 1.00 50.66	0
MOTA	2408 NE2 GLN A 330	7.621 62.489 112.507 1.00 52.87	N
MOTA	2409 N LEU A 331	9.146 59.231 117.017 1.00 40.46	N
ATOM	2410 CA LEU A 331	10.191 59.526 117.961 1.00 44.60	C
MOTA	2411 C LEU A 331	11.053 60.640 117.399 1.00 49.33	Ċ
ATOM	2412 O LEU A 331	11.194 61.701 118.016 1.00 52.75	0
ATOM	2413 CB LEU A 331	11.037 58.283 118.216 1.00 45.31	C
MOTA	2414 CG LEU A 331	12.287 58.486 119.082 1.00 48.54	c
MOTA	2415 CD1 LEU A 331	12.005 59.479 120.190 1.00 55.41	C
ATOM	2416 CD2 LEU A 331	12.735 57.150 119.650 1.00 52.33	C
MOTA	2417 N ARG A 332	11.603 60.400 116.211 1.00 53.70	N
MOTA	2418 CA ARG A 332	12.473 61.361 115.550 1.00 60.63	C
MOTA	2419 C ARG A 332	11.950 62.002 114.262 1.00 60.77	C
MOTA MOTA	2420 O ARG A 332	11.004 61.528 113.632 1.00 55.57	0
NION	2421 CB ARG A 332	13.826 60.707 115.267 1.00 65.11	С

ATOM	2422	CG	ARC	A 332	14.770	60.696 116.450	1.00 69.71	С
							1.00 69.46	
MOTA	2423	CĐ		A 332	16.044	59.921 116.147		С
MOTA	2424	NE	ARG A	A 332	17.140	60.259 117.057	1.00 75.06	N
ATOM	2425	CZ	ARG A	A 332	17.059	60.232 118.384	1.00 81.31	С
ATOM	2426	NH1	ARG A		15.927	59.882 118.981	1.00 82.93	N
MOTA	2427		ARG A		18.112	60.563 119.120	1.00 85.14	N
MOTA	2428	N	GLN A	A 333	12.610	63.092 113.890	1.00 65.78	N
ATOM	2429	CA	GLN A	A 333	12.296	63.855 112.701	1.00 67.90	С
ATOM	2430	С		A 333	13.634	64.097 112.058	1.00 71.18	č
MOTA	2431	0		A 333	14.632	63.535 112.479	1.00 68.31	0
ATOM	2432	CB	GLN A	A 333	11.707	65.201 113.085	1.00 72.61	С
ATOM	2433	CG	GLN A	A 333	10.993	65.880 111.956	1.00 79.18	С
ATOM	2434	CD	GLN A		9.729	65.146 111.594	1.00 86.56	č
ATOM	2435		GLN A		9.004	65.538 110.685	1.00 93.40	0
ATOM	2436	NES	GLN A	4 333	9.455	64.067 112.312	1.00 88.10	N
ATOM	2437	N	GLY A	334	13.655	64.945 111.042	1.00 79.40	N
ATOM	2438	CA	GLY A	334	14.909	65.269 110.384	1.00 87.47	С
ATOM	2439	C	GLY A		15.453	64.373 109.285	1.00 87.45	č
MOTA	2440	0	GLY A		15.146	63.179 109.202	1.00 84.44	٠ ٥
ATOM	2441	N	ASP A	1 335	16.284	64.982 108.440	1.00 88.86	N
ATOM	2442	CA	ASP A	A 335	16.920	64.309 107.308	1.00 85.39	C
ATOM	2443	С	ASP A	335	15.968	63.347 106.612	1.00 77.33	С
ATOM	2444	ō	ASP A		16.228	62.146 106.544	1.00 74.37	ō
ATOM	2445	CB	ASP A		18.159	63.544 107.778	1.00 95.54	C
MOTA	2446	CG	ASP A	1 335	19.155	63.309 106.661	1.00100.21	С
MOTA	2447	ODl	ASP A	335	19.861	64.273 106.289	1.00102.26	0
MOTA	2448	OD2	ASP A	1 335	19.224	62.168 106.150	1.00104.80	0
ATOM	2449	N	ASN A		14.874	63.890 106.088	1.00 69.33	- N
MOTA	2450	CA	ASN A		13.866	63.090 105.411	1.00 62.56	С
ATOM	2451	Ç	ASN A	336	13.805	61.697 105.990	1.00 56.64	С
ATOM	2452	0	ASN A	336	13.968	60.706 105.285	1.00 56.81	0
ATOM	2453	CB	ASN A		14.153	63.021 103.920	1.00 64.42	Ċ
ATOM	2454	CG	ASN A					č
					13.485	64.129 103.172	1.00 75.47	
ATOM	2455		ASN A		12.306	64.400 103.395	1.00 80.59	0
ATOM	2456	ND2	ASN A	336	14.220	64.782 102.277	1.00 82.36	N
ATOM	2457	N	PHE A	337	13.562	61.636 107.291	1.00 45.38	N
MOTA	2458	CA		337	13.502	60.373 107.986	1.00 32.52	C
ATOM	2459	Ċ	PHE A		12.569	60.501 109.172	1.00 31.65	
								C
ATOM	2460	0		337	12.612	61.499 109.890	1.00 41.04	0
ATOM	2461	CB	PHE A	337	14.901	59.984 108.464	1.00 35.90	С
MOTA	2462	CG	PHE A	337	15.625	59.044 107.538	1.00 41.00	С
ATOM	2463		PHE A		16.977	59.219 107.268	1.00 43.16	Ċ
ATOM	2464		PHE A		14.966	57.962 106.962	1.00 43.25	č
ATOM	2465			337	17.666	58.331 106.440	1.00 46.01	c c
ATOM	2466	CE2	PHE A	337	15.644	57.072 106.136	1.00 45.63	С
ATOM	2467	CZ	PHE P	337	16.999	57.257 105.874	1.00 45.74	С
ATOM	2468	N	GLU A	338	11.716	59.502 109.367	1.00 26.29	N
ATOM	2469	CA	GLU A		10.786	59.502 110.481	1.00 29.69	Ċ
								Č
ATOM	2470	Č	GLU A		10.962	58.218 111.252	1.00 23.34	c
ATOM	2471	0	GLU A		10.997	57.150 110.656	1.00 27.49	0
ATOM	2472	CB	GLU A	338	9.343	59.581 109.980	1.00 34.11	C
MOTA	2473	CG	GLU A	338	8.840	60.986 109.680	1.00 38.07	С
ATOM	2474	CD	GLU A		7.316	61.070 109.589	1.00 43.85	Ċ
ATOM	2475		GLU A		6.625	60.777 110.597	1.00 46.32	ŏ
ATOM	2476		GLU A		6.809	61.436 108.508	1.00 47.89	0
ATOM	2477	N	VAL A	339	11.067	58.304 112.572	1.00 12.61	N
ATOM	2478	CA	VAL A	339	11.209	57.093 113.363	1.00 12.26	С
ATOM	2479	С	VAL A		10.028	56.913 114.297	1.00 9.82	Ċ
ATOM	2480	ŏ	VAL A		9.867	57.674 115.257	1.00 17.52	ŏ
		-				57.113 114.214		c
MOTA	2481	CB	VAL A		12.488		1.00 16.72	Ċ
MOTA	2482		VAL A		12.474	55.945 115.191	1.00 18.37	C
ATOM	2483	CG2	VAL A	339	13.712	57.046 113.318	1.00 24.35	С
ATOM	2484	N	TRP A	340	9.209	55.902 114.035	1.00 9.60	N
ATOM	2485	ÇA	TRP A		8.056	55.644 114.889	1.00 17.16	C
								č
ATOM	2486	C	TRP A		8.305	54.434 115.790	1.00 17.17	č
ATOM	2487	0_	TRP A		9.208	53.638 115.532	1.00 16.55	0
ATOM	2488	CB	TRP A		6.816	55.416 114.029	1.00 25.15	C
ATOM	2489	CG	TRP A	340	6.367	56.646 113.324	1.00 32.90	С
ATOM	2490		TRP A		7.086	57.387 112.440	1.00 33.98	С
ATOM	2491		TRP A		5.110	57.309 113.473	1.00 41.04	č
ATOM	2492		TRP A		6.358	58.475 112.026	1.00 42.03	N
MOTA	2493		TRP A		5.140	58.452 112.644	1.00 46.80	c c
ATOM	2494	CE3	TRP A	340	3.961	57.051 114.226	1.00 47.74	С
ATOM	2495		TRP A		4.070	59.338 112.550	1.00 56.89	С
ATOM	2496		TRP A		2.896	57.933 114.134	1.00 47.15	č
ATOM	2497		TRP A		2.958	59.064 113.300	1.00 55.77	č
ATOM	2498	N	GLU A		7.513	54.304 116.852	1.00 16.97	N
MOTA	2499	CA	GLU A		7.650	53.182 117.784	1.00 17.90	С
MOTA	2500	С	GLU A	341	6.443	53.057 118.719	1.00 15.85	С
ATOM	2501	0	GLU A		5.845	54.049 119.150	1.00 17.73	0
ATOM	2502	CB.	GLU A		8.919	53.329 118.632	1.00 18.18	č
	-302	CD	350 8	41	0.313	JJ.JEJ 110.0JE	1.00 10.10	C

3001	2502	~~								36 50	_
ATOM	2503	CG	GLU			8.721		119.882		36.58	c
ATOM	2504	CD	GLU			10.016		120.644		40.66	Ċ
ATOM	2505	0E1	GLU	Α	341	10.732	53.440	120.940	1.00	43.84	0
MOTA	2506	OE2	GLU	Α	341	10.323	55.586	120.963	1.00	45.95	0
ATOM	2507	N	ARG			6.099		119.028		20.21	N
ATOM	2508	CA	ARG			4.985		119.908		27.65	Č
ATOM	2509	С	ARG	Α	342	5.438	50.477	120.918	1.00	31.87	С
MOTA	2510	0	ARG	А	342	6.049	49.473	120.545	1.00	42.57	0
MOTA	2511	CB	ARG			3.800		119.105		25.33	С
											č
ATOM	2512	CG	ARG			2.701		119.985		25.09	Ċ
ATOM	2513	CD	ARG	Α	342	1.752	49.448	119.237	1.00	24.25	С
MOTA	2514	NE	ARG	Α	342	0.577	49.103	120.044	1.00	26.47	N
ATOM	2515	CZ	ARG			-0.452		119.598		30.27	С
											N
ATOM	2516		ARG			-0.440		118.353		31.99	
MOTA	2517	NH 2	ARG			-1.506		120.371		34.96	N
MOTA	2518	N	PRO	Α	343	5.181	50.702	122.211	1.00	26.00	N
MOTA	2519	CA	PRO	Δ	343	5.611	49 668	123.148	1 00	21.89	С
ATOM	2520	c.	PRO			4.547		123.068		27.99	č
MOTA	2521	0	PRO			3.358		122.905		26.98	Ō
MOTA	2522	CB	PRO	Α	343	5.603	50.396	124.474	1.00	8.64	С
MOTA	2523	ÇG	PRO	Α	343	4.455	51.318	124.316	1.00	11.85	С
MOTA	2524	CD	PRO			4.640		122.923		20.11	Ċ
											Ň
ATOM	2525	N	LEU			4.970		123.156		34.97	
MOTA	2526	CA	LEU	Α	344	4.040		123.085		39.22	С
MOTA	2527	С	LEU	Α	344	3.918	45.574	124.477	1.00	46.77	С
ATOM	2528	ō	LEU			4.025		125.478		51.96	Ō
	2529	ČВ	LEU			4.570		122.098		30.94	č
ATOM											č
MOTA	2530	CG	LEU			5.077		120.842		35.48	0000
MOTA	2531	CD1	LEU	Α	344	5.746	44.857	119.914	1.00	43.68	С
MOTA	2532	CD2	LEU	Α	344	3.902	46.557	120.172	1.00	44.42	С
ATOM	2533	N	SER			3.690		124.535		51.33	N
						3.577				57.81	
MOTA	2534	CA	SER					125.805			C
MOTA	2535	С	SER	Α	345	4.868		125.989	1.00	57.31	C
MOTA	2536	0	SER	Α	345	5.555	42.511	125.015	1.00	54.00	0
ATOM	2537	CB	SER	Α	345	2.399	42.602	125.776	1.00	65.41	С
MOTA	2538	ŌĞ	SER			1.220		125.356		72.59	Ō
										58.68	
MOTA	2539	N	GLY			5.203		127.233			N
MOTA	2540	CA	GLY			6.409		127.507	1.00	63.75	С
MOTA	2541	С	GLY	Α	346	7.730	42.381	127.180	1.00	66.32	С
MOTA	2542	0	GLY			8.646	41.720	126.694	1.00	68.08	0
	2543	Ň	LEU			7.831		127.446		67.45	N
ATOM											
ATOM	2544	CA	LEU			9.061		127.194		70.86	Ç
MOTA	2545	С	LEU	А	347	9.484	44.433	125.727	1.00	71.91	С
MOTA	2546	0	LEU	Α	347	10.639	44.721	125.398	1.00	78.43	0
ATOM	2547	ČВ	LEU			10.196		128.049		77.11	С
											č
MOTA	2548	CG	LEU			9.956		129.559		85.78	· ·
ATOM	2549	CD1	LEU	Α	347	11.102	43.153	130.256	1.00	94.76	С
ATOM	2550	CD2	LEU	Α	347	9.829	45.302	130.055	1.00	88.27	С
ATOM	2551	N	ALA			8.543		124.853	1.00	66.88	N
	2552	CA	ALA			8.804		123.427		55.04	Ċ
ATOM											
ATOM	2553	С			348	8.354		122.809		41.31	c
ATOM	2554	0	ALA	Α	348	7.332	45.923	123.196		35.51	0
ATOM	2555	CB	ALA	Α	348	8.062	42.893	122.797	1.00	67.28	С
ATOM	2556	N	TRP			9.124		121.850		32.83	N
ATOM	2557	CA	TRP			8.785		121.202		27.38	c
АТОМ	2558	С	TRP	Α	349	8.779		119.687		28.15	С
ATOM	2559	0	TRP	Α	349	9.598	46.318	119.095	1.00	30.66	0
ATOM	2560	CB	TRP			9.769		121.622		27.05	С
ATOM	2561	CG	TRP			9.634		123.031		26.81	č
MOTA	2562		TRP			9.686		124.145		38.79	c
ATOM	2563	CD2	TRP	Α	349	9.489	49.947	123.505	1.00	19.14	С
ATOM	2564	NE1	TRP	А	349	9.586	48.572	125.285	1.00	34.04	N
ATOM	2565		TRP			9.464		124.920		28.66	С
	2566					9.380		122.875		11.37	č
ATOM			TRP								_
ATOM	2567	CZ2	TRP	Α	349	9.335		125.711		36.09	С
ATOM	2568	CZ3	TRP	Α	349	9.254	52.320	123.649	1.00	29.51	Ċ
MOTA	2569		TRP			9.232		125.057	1.00	39.76	С
ATOM	2570	N	ALA			7.847		119.064		24.57	N
ATOM	2571	CA	ALA			7.735		117.612		24.86	c
MOTA	2572	С	ALA			8.318		117.157		28.08	c
MOTA	2573	0	ALA	Α	350	8.108	50.125	117.814	1.00	35.08	0
MOTA	2574	СB	ALA			6.273		117.203		24.91	С
ATOM	2575	N	VAL			9.049		116.042		28.62	N
ATOM	2576	CA	VAL			9.657		115.537		29.07	c
MOTA	2577	С	VAL	Α	351	9.529		114.028		32.11	С
MOTA	2578	0	VAL	Α	351	9.734	49.573	113.253	1.00	31.37	0
MOTA	2579	СB	VAL			11.156		115.887		30.43	Ċ
								115.487		26.13	č
ATOM	2580		VAL			11.696					Ċ
ATOM	2581		VAL			11.367		117.365		22.49	
MOTA	2582	N	ALA			9.217		113.617		28.58	N
MOTA	2583	CA	ALA	Α	352	9.055	52.060	112.199	1.00	29.67	С

2588 CA MET A 353 11.5: 2589 C MET A 353 11.0: 2590 O MET A 353 11.0: 2591 CB MET A 353 12.7: 2592 CG MET A 353 13.9: 2593 SD MET A 353 14.8: 2594 CE MET A 353 15.4' 2595 N ILE A 354 10.5: 2596 CA ILE A 354 11.00 2597 C ILE A 354 11.5: 2599 CB ILE A 354 11.5: 2599 CB ILE A 354 7.8: 2600 CG1 ILE A 354 8.7' 2600 CG1 ILE A 354 8.7' 2601 CG2 ILE A 354 8.0' 2602 CD1 ILE A 354 8.0' 2603 N ASN A 355 11.2: 2605 C ASN A 355 12.1: 2605 C ASN A 355 11.2: 2606 O ASN A 355 11.2: 2606 O ASN A 355 11.2: 2607 CB ASN A 355 11.2: 2608 CG ASN A 355 11.2: 2608 CG ASN A 355 11.2: 2609 OD1 ASN A 355 13.0! 2611 N ARG A 356 10.5: 2612 CA ARG A 356 10.2: 2613 C ARG A 356 10.5: 2614 O ARG A 356 10.5: 2615 CB ARG A 356 6.0: 2617 CD ARG A 356 10.5: 2618 NE ARG A 356 6.0: 2620 NH1 ARG A 356 6.0: 2621 NH2 ARG A 356 6.0: 2622 N GLN A 357 12.6: 2624 C GLN A 357 12.6: 2625 O GLN A 357 12.6: 2626 CB GLN A 357 12.6: 2627 CG GLN A 357 12.6: 2628 CD GLN A 357 12.6: 2629 OE1 GLN A 357 12.6: 2629 OE1 GLN A 357 12.6: 2621 CA GLN A 357 12.6: 2622 CG GLN A 357 12.6: 2624 C GLN A 357 12.6: 2625 O GLN A 357 12.6: 2626 CB GLN A 357 14.1! 2627 CG GLN A 357 12.6: 2628 CD GLN A 357 14.1! 2627 CG GLN A 357 12.6: 2629 OE1 GLN A 357 12.6: 2620 CB GLN A 357 12.6: 2621 CA GLN A 357 12.6: 2622 CD GLN A 357 12.6: 2623 CA GLN A 357 12.6: 2624 C GLN A 357 12.6: 2625 O GLN A 357 12.6: 2626 CB GLN A 357 12.6: 2627 CG GLN A 357 12.6: 2628 CD GLN A 357 12.6: 2629 OE1 GLN A 357 12.6: 2629 OE1 GLN A 357 12.6: 2620 NH1 ARG A 358 10.5: 2631 C GLU A 358 10.5: 2632 CA GLU A 358 10.5: 2634 O GLU A 358 10.5: 2635 CB GLU A 358 10.5: 2636 CB GLU A 358 10.5: 2637 CD GLU A 358 10.5: 2638 OE1 GLU A 358 10.5: 2639 OE2 GLU A 358 10.5: 2630 CB GLU A 358 10.5: 2631 CB GLU A 358 10.5: 2632 CA GLU A 358 10.5: 2633 CA GLU A 358 10.5: 2634 O GLU A 358 10.5: 2635 CB GLU A 358 10.5: 2636 CB GLU A 358 10.5: 2637 CD GLU A 358 10.5: 2638 OE1 GLU A 358 10.5: 2639 OE2 GLU A 358 10.5: 2630 CB GLU A 358 10.5: 2631 CB GLU A 358 10.5: 2631 CB GLU A 358 10.5: 2632 CB GLU A 358 10.5: 2634 CB GLU A 358 10
C MET A 353 11.00 O MET A 353 11.01 CB MET A 353 12.75 CG MET A 353 12.75 CG MET A 353 13.97 SD MET A 353 14.85 CE MET A 353 15.45 N ILE A 354 10.06 C ILE A 354 11.06 O ILE A 354 11.06 O ILE A 354 11.06 C ILE A 355 11.26 CB ILE A 355 11.26 CB ILE A 355 12.15 CC ASN A 355 12.15 CA ASN A 355 12.15 CA ASN A 355 11.26 CA ASN A 355 11.26 CB ASN A 355 11.26 CB ASN A 355 10.76 CG ASN A 355 10.76 CC ARG A 356 10.96 O ARG A 356 10.96 O ARG A 356 6.66 CZ ARG A 356 6.66 CZ ARG A 356 6.61 NH1 ARG A 356 6.61 NH1 ARG A 356 6.61 NH2 ARG A 356 6.61 NH2 ARG A 356 6.61 NH4 ARG A 357 12.66 CC ARG A 357 12.66 CC ALN A 357 12.66 CC GLU A 358 10.57 CD GLN A 357 12.66 CC GLU A 358 10.57 CC GLU A 358 10.56 CC GLU A 358 10.66 CC GLU A
MET A 353 11.00 MET A 353 12.11 MET A 353 12.21 MET A 353 13.99 MET A 353 14.80 MET A 353 15.41 ILE A 354 10.00 ILE A 354 11.00 ILE A 355 11.20 ASN A 355 11.21 ASN A 355 11.22 ASN A 355 11.23 ASN A 355 11.24 ASN A 355 11.25 ASN A 355 11.26 ASN A 355 10.77 ASN A 355 13.80 ASN A 355 13.8
353
11.0: 11.1: 12.7: 14.8: 15.4: 10.0: 11
31971730014780015571218279964714735417785160318857572556488155703754696790
53.576 53.576 53.2748 53.367 52.208 53.367 52.708 55.669 55.669 55.756 56.393 57.8190 57.8
100.456 99.090 98.540 100.585 99.464 99.914 100.755 99.359 98.552 97.275 96.072 95.132 96.817 99.012 96.817 99.012 96.817 99.012 96.90 94.961 95.320 96.485 92.951 95.206 94.306 94.538 94.690 92.160 94.306 94.538 94.690 93.918 95.692 95.919 97.395 98.152 97.842 99.246
1.00 1.00
21. 96 24. 69 24. 69 25. 69 26. 69 27. 80 28. 71 29. 46 20. 54 20. 54

MOTA	2665	С	ARG	Δ	363	19.375	54 587	103.018	1.00	46.90	С
MOTA	2666	ŏ	ARG			18.713		103.150	1.00		ŏ
ATOM	2667	СВ				18.664			1.00		č
			ARG					102.217	1.00		č
MOTA	2668	CC	ARG			18.232		100.992			
ATOM	2669	CD	ARG			18.212		101.160		50.08	C
MOTA	2670	NE	ARG			17.069		101.936		60.37	N
MOTA	2671	CZ	ARG			17.117		103.238		67.25	C
MOTA	2672		ARG			18.257		103.895		62.40	N
MOTA	2673		ARG			16.035		103.881		78.35	N
MOTA	2674	N	SER			20.322		103.874	1.00		N
MOTA	2675	CA	SER	Α	364	20.572	54.123	105.046	1.00		С
ATOM	2676	С	SER			20.457		106.297		54.18	С
MOTA	2677	0	SER	Α	364	20.946	56.093	106.341	1.00		0
MOTA	2678	CB	SER	Α	364	21.958	53.479	104.976	1.00	59.39	С
MOTA	2679	OG	SER	Α	364	22.984	54.452	104.893	1.00	72.85	0
MOTA	2680	N	TYR	Α	365	19.780	54.429	107.303	1.00	55.27	N
MOTA	2681	CA	TYR	Α	365	19.621	55.135	108.557	1.00	57.93	С
MOTA	2682	C	TYR	Α	365	20.214	54.282	109.674	1.00	57.07	С
MOTA	2683	0	TYR	Α	365	20.069	53.058	109.685	1.00	56.96	0
MOTA	2684	CB	TYR	Α	365	18.147	55.431	108.832	1.00	57.81	С
ATOM	2685	CG	TYR			17.963		109.937		64.43	С
MOTA	2686		TYR			18.372		109.769	1.00	72.40	С
ATOM	2687		TYR			17.428		111.179		65.59	c c c
ATOM	2688	CEI				18.257		110.814		77.79	č
ATOM	2689		TYR			17.308		112.233		62.72	č
MOTA	2690	cz	TYR			17.725		112.047		69.04	č
	2691	ОН	TYR			17.618		113.080		60.28	ŏ
MOTA	2692	N	THR			20.887		110.606		54.01	N
MOTA			THR			21.532		111.729		50.62	Č
ATOM	2693	CA									č
ATOM		C	THR			21.223		113.036		51.78	
MOTA		0	THR			21.341		113.105		61.83	0
MOTA		CB	THR			23.050		111.539		47.56	Č
MOTA			THR			23.489		111.339		54.98	0
ATOM			THR			23.442		110.331		37.27	c
MOTA		N	ILE			20.828		114.070		44.35	N
MOTA		CA	ILE			20.538		115.377		43.01	C C
MOTA		С	ILE		-	21.113		116.562		44.48	C
MOTA		0	ILE			21.527		116.437		51.46	0
MOTA		CB	ILE			19.031		115.657		46.14	Č
MOTA	2704	CG1	ILE	Α	367	18.284		115.204		46.40	C
MOTA	2705	CG2	ILE	Α	367	18.515		115.022		55.17	Ċ
MOTA	2706	CD1	ILE	Α	367	18.671	52.535	115.960	1.00	50.08	Ċ
MOTA	2707	N	ALA	Α	368	21.120	54.780	117.716	1.00	46.92	N
MOTA	2708	CA	ALA	Α	368	21.628	54.182	118.937	1.00	53.37	С
MOTA	2709	С	ALA	Α	368	20.604	53.228	119.552	1.00	52.95	С
MOTA	2710	0	ALA	Α	368	19.672	53.648	120.233	1.00	55.58	0
ATOM		СВ	ALA			21.999	55.279	119.932	1.00	64.28	С
ATOM		N	VAL			20.790	51.943	119.283	1.00	46.01	N
ATOM		CA	VAL			19.939		119.813	1.00	36.78	С
ATOM		Ċ	VAL			19.413		121.187		31.16	C
ATOM		ŏ	VAL			18.230		121.502		23.65	0
ATOM		ČВ	VAL			20.748		119.955		46.22	С
ATOM			VAL			19.984		120.738		49.54	С
MOTA			VAL			21.109		118.585		57.99	č
ATOM		N	ALA			20.312		122.005		37.15	N
MOTA		CA	ALA			19.975		123.356		46.82	Ċ
MOTA		c	ALA			18.860		123.383		49.03	č
ATOM		ŏ	ALA			17.741		123.794		54.27	ō
ATOM	2723	СВ				21.219		124.044		53.44	č
-			ALA SER			19.171		122.932		46.02	N
MOTA		N						122.930		49.13	ĉ
MOTA		CA	SER			18.196					č
MOTA		C	SER			17.016		122.018		46.74 51.75	o
ATOM	2727	0	SER			16.569		121.285	1.00		č
					3/1		E 6 000	122 515	1 00		
MOTA	2728	CB	SER			18.861		122.515	1.00		
MOTA MOTA	2728 2729	OG	SER	Α	371	19.222	56.878	121.148	1.00	46.67	. 0
MOTA MOTA MOTA	2728 2729 2730	OG N	SER LEU	A A	371 372	19.222 16.511	56.878 54.038	121.148 122.072	1.00 1.00	46.67 43.25	. O N
MOTA MOTA MOTA MOTA	2728 2729 2730 2731	OG N CA	SER LEU LEU	A A A	371 372 372	19.222 16.511 15.377	56.878 54.038 53.651	121.148 122.072 121.242	1.00 1.00 1.00	46.67 43.25 39.52	. O N C
MOTA MOTA MOTA MOTA MOTA	2728 2729 2730 2731 2732	OG N CA C	SER LEU LEU LEU	A A A	371 372 372 372	19.222 16.511 15.377 14.135	56.878 54.038 53.651 53.415	121.148 122.072 121.242 122.092	1.00 1.00 1.00 1.00	46.67 43.25 39.52 41.63	. О И С С
MOTA MOTA MOTA MOTA MOTA MOTA	2728 2729 2730 2731 2732 2733	OG N CA C	SER LEU LEU LEU LEU	A A A A	371 372 372 372 372 372	19.222 16.511 15.377 14.135 13.319	56.878 54.038 53.651 53.415 54.321	121.148 122.072 121.242 122.092 122.285	1.00 1.00 1.00 1.00 1.00	46.67 43.25 39.52 41.63 43.63	. O N C C
MOTA MOTA MOTA MOTA MOTA MOTA MOTA	2728 2729 2730 2731 2732 2733 2734	OG N CA C O CB	SER LEU LEU LEU LEU LEU	A A A A A	371 372 372 372 372 372 372	19.222 16.511 15.377 14.135 13.319 15.698	56.878 54.038 53.651 53.415 54.321 52.382	121.148 122.072 121.242 122.092 122.285 120.440	1.00 1.00 1.00 1.00 1.00	46.67 43.25 39.52 41.63 43.63 38.36	. O N C C O C
MOTA ATOM ATOM ATOM ATOM ATOM AOTA MOTA M	2728 2729 2730 2731 2732 2733 2734 2735	OG N CA C O CB CG	SER LEU LEU LEU LEU LEU LEU	A A A A A	371 372 372 372 372 372 372 372	19.222 16.511 15.377 14.135 13.319 15.698 14.636	56.878 54.038 53.651 53.415 54.321 52.382 51.986	121.148 122.072 121.242 122.092 122.285 120.440 119.403	1.00 1.00 1.00 1.00 1.00 1.00	46.67 43.25 39.52 41.63 43.63 38.36 39.85	. O N C C O C
MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA	2728 2729 2730 2731 2732 2733 2734 2735 2736	OG N CA C O CB CG CD1	SER LEU LEU LEU LEU LEU LEU	A A A A A A A	371 372 372 372 372 372 372 372 372	19.222 16.511 15.377 14.135 13.319 15.698 14.636 14.260	56.878 54.038 53.651 53.415 54.321 52.382 51.986 53.182	121.148 122.072 121.242 122.092 122.285 120.440 119.403 118.536	1.00 1.00 1.00 1.00 1.00 1.00 1.00	46.67 43.25 39.52 41.63 43.63 38.36 39.85 35.69	. O N C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2728 2729 2730 2731 2732 2733 2734 2735 2736 2737	OG N CA C O CB CG CD1 CD2	SER LEU LEU LEU LEU LEU LEU LEU	A A A A A A A	371 372 372 372 372 372 372 372 372 372	19.222 16.511 15.377 14.135 13.319 15.698 14.636 14.260 15.169	56.878 54.038 53.651 53.415 54.321 52.382 51.986 53.182 50.868	121.148 122.072 121.242 122.092 122.285 120.440 119.403 118.536 118.528	1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	46.67 43.25 39.52 41.63 43.63 38.36 39.85 35.69 33.08	. O N C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2728 2729 2730 2731 2732 2733 2734 2735 2736 2737 2738	OG N CA C O CB CG CD1 CD2 N	SER LEU LEU LEU LEU LEU LEU LEU GLY	A A A A A A A A	371 372 372 372 372 372 372 372 372 372 373	19.222 16.511 15.377 14.135 13.319 15.698 14.636 14.260 15.169 13.995	56.878 54.038 53.651 53.415 54.321 52.382 51.986 53.182 50.868 52.190	121.148 122.072 121.242 122.092 122.285 120.440 119.403 118.536 118.528 122.596	1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	46.67 43.25 39.52 41.63 43.63 38.36 39.85 35.69 33.08 41.36	. 0 0 0 0 0 0 0 0 0 0
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2728 2729 2730 2731 2732 2733 2734 2735 2736 2737 2738 2739	OG N CA C O CB CG CD1 CD2 N CA	SER LEU LEU LEU LEU LEU LEU GLY GLY	A A A A A A A A A A A A A A A A A A A	371 372 372 372 372 372 372 372 372 373 373	19.222 16.511 15.377 14.135 13.319 15.698 14.636 14.260 15.169 13.995 12.847	56.878 54.038 53.651 53.415 54.321 52.382 51.986 53.182 50.868 52.190 51.847	121.148 122.072 121.242 122.092 122.285 120.440 119.403 118.536 118.528 122.596 123.423	1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	46.67 43.25 39.52 41.63 43.63 38.36 39.85 35.69 33.08 41.36 42.44	. O N C C C C C C C N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2728 2729 2730 2731 2732 2733 2734 2735 2736 2737 2738 2739 2740	OG N CA C O CB CG CD1 CD2 N CA C	SER LEU LEU LEU LEU LEU LEU GLY GLY GLY	A A A A A A A A A A A	371 372 372 372 372 372 372 372 372 373 373	19.222 16.511 15.377 14.135 13.319 15.698 14.636 14.260 15.169 13.995 12.847 12.892	56.878 54.038 53.651 53.415 54.321 52.382 51.986 53.182 50.868 52.190 51.847 52.616	121.148 122.072 121.242 122.092 122.285 120.440 119.403 118.536 118.528 122.596 123.423 124.718	1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	46.67 43.25 39.52 41.63 43.63 38.36 39.85 35.69 33.08 41.36 42.44 43.08	. 0 N C C C C C C N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2728 2729 2730 2731 2732 2733 2734 2735 2736 2737 2738 2739 2740 2741	OG N CA C O CB CG CD1 CD2 N CA C	SER LEU LEU LEU LEU LEU LEU GLY GLY GLY GLY	A A A A A A A A A A A A A A A A A A A	371 372 372 372 372 372 372 372 372 373 373	19.222 16.511 15.377 14.135 13.319 15.698 14.636 14.260 15.169 13.995 12.847 12.892 12.973	56.878 54.038 53.651 53.415 54.321 52.382 51.986 53.182 50.868 52.190 51.847 52.616 52.027	121.148 122.072 121.242 122.092 122.285 120.440 119.403 118.536 118.528 122.596 123.423 124.718 125.792	1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	46.67 43.25 39.52 41.63 43.63 38.36 39.85 35.69 33.08 41.36 42.44 43.08 41.04	. NN CC CC CC NN CC CO
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2728 2729 2730 2731 2732 2733 2734 2736 2737 2738 2739 2740 2741	OG N CA C O CB CG CD1 CD2 N CA C	SER LEU LEU LEU LEU LEU LEU GLY GLY GLY LYS	A A A A A A A A A A A A A A A A	371 372 372 372 372 372 372 372 373 373 373	19.222 16.511 15.377 14.135 13.319 15.698 14.260 14.260 15.169 13.995 12.847 12.892 12.892	56.878 54.038 53.651 53.415 54.321 52.382 51.986 53.182 50.868 52.190 51.847 52.616 52.027 53.940	121.148 122.072 121.242 122.092 122.285 120.440 119.403 118.536 118.528 122.596 123.423 124.718 125.792 124.601	1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	46.67 43.25 39.52 41.63 43.63 38.36 39.85 35.69 33.08 41.36 42.44 43.08 41.04 42.62	. O . N . C . C . C . C . C . C . C . C . C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2728 2729 2730 2731 2732 2733 2734 2735 2736 2737 2738 2739 2740 2741 2741 2743	OG N CA C O CB CG CD1 CD2 N CA C	SER LEU LEU LEU LEU LEU LEU LEU GLY GLY GLY LYS LYS	A A A A A A A A A A A A A A A	371 372 372 372 372 372 372 372 372 373 373	19.222 16.511 15.377 14.135 13.319 15.698 14.636 14.260 15.169 13.995 13.995 12.892 12.892 12.973	56.878 54.038 53.651 53.415 54.321 52.382 51.986 53.182 50.868 52.190 51.847 52.616 52.027 53.940 54.836	121.148 122.072 121.242 122.092 122.285 120.440 119.403 118.536 118.528 122.596 123.423 124.718 125.792 124.601 125.745	1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	46.67 43.25 39.52 41.63 43.63 38.36 39.85 35.69 33.08 41.36 42.44 43.08 41.04 42.62 40.40	. O N C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2728 2729 2730 2731 2732 2733 2734 2735 2736 2737 2738 2740 2741 2742 2743	OG N CA C O CB CG CD1 CD2 N CA C	SER LEU LEU LEU LEU LEU LEU GLY GLY GLY LYS	A A A A A A A A A A A A A A	371 372 372 372 372 372 372 372 373 373 373	19.222 16.511 15.377 14.135 13.319 15.698 14.260 14.260 15.169 13.995 12.847 12.892 12.892	56.878 54.038 53.651 53.415 54.321 52.382 51.986 53.182 50.868 52.190 51.847 52.616 52.027 53.940 54.836 54.461	121.148 122.072 121.242 122.092 122.285 120.440 119.403 118.536 118.528 122.596 123.423 124.718 125.792 124.601	1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	46.67 43.25 39.52 41.63 43.63 38.36 39.85 35.69 33.08 41.36 42.44 43.08 41.04 42.62	. O . N . C . C . C . C . C . C . C . C . C

АТОМ	2746	CB	LYS			11.596		126.528	1.00 43.36		c
ATOM ATOM	2747 2748	CG CD	LYS	A	374 374	10.897 9.446		126.618	1.00 55.37 1.00 70.29		C
ATOM	2749	CE	LYS		374	8.697		127.032 126.997	1.00 76.29		č
ATOM	2750	NZ	LYS			8.656		125.628	1.00 85.28		N
MOTA	2751	N	GLY			15.026	53.724	126.085	1.00 46.09		N
ATOM	2752	CA	GLY		375	16.187		126.843	1.00 45.98		C
ATOM ATOM	2753 2754	C 0	GLY		375 375	16.051 17.045		127.397 127.567	1.00 44.25 1.00 42.54		C 0
MOTA	2755	N	VAL			14.815		127.670	1.00 44.63		N
MOTA	2756	CA	VAL		376	14.521		128.213	1.00 48.90		С
MOTA	2757	C	VAL		376	14.846		127.261	1.00 51.39		C
MOTA	2758	0	VAL			15.870		127.426	1.00 60.38		0
MOTA MOTA	2759 2760	CB	VAL		376 376	13.044 12.742		128.596 129.011	1.00 56.12		c
ATOM	2761		VAL		376	12.723		129.715	1.00 60.19		č
MOTA	2762	N	ALA		377	13.965		126.289	1.00 48.99		N
MOTA	2763	CA	ALA			14.176		125.322	1.00 50.51		C
MOTA	2764	C	ALA		377	15.583		124.777	1.00 50.00		C 0
ATOM ATOM	2765 2766	O CB	ALA ALA		377	15.931 13.170		124.181 124.202	1.00 43.03 1.00 55.85		Č
MOTA	2767	N	CYS		378	16.381		125.012	1.00 54.41		N
MOTA	2768	CA	CYS		378	17.788		124.606	1.00 63.17		С
MOTA	2769	C	CYS		378	18.736		125.791	1.00 64.43		C
MOTA MOTA	2770 2771	O CB	CYS		378 378	19.948 18.160		125.618 123.647	1.00 68.38		0
MOTA	2772	SG	CYS			17.553		121.960	1.00 65.15		S
ATOM	2773	N	ASN		379	18.193		126.991	1.00 61.33		N
MOTA	2774	CA	ASN		379	19.024		128.192	1.00 63.54		С
MOTA	2775	Ċ	ASN		379	18.918		128.858	1.00 65.33		C
ATOM	2776 2777	O CB	ASN		379 379	17.886 18.571		129.434 129.172	1.00 62.68 1.00 71.26		0
ATOM ATOM	2778	CG	ASN		379	19.666		130.157	1.00 81.14		Č
ATOM	2779	OD1			379	20.752		129.749	1.00 80.80		0
MOTA	2780	ND2	ASN		379	19.393		131.453	1.00 90.99		N
ATOM	2781	N	PRO		380	19.978		128.752	1.00 65.49		N C
ATOM ATOM	2782 2783	CA C	PRO PRO		380 380	21.210 21.125		128.042 126.655	1.00 68.72 1.00 71.25		
ATOM	2784	ò	PRO		380	21.714		125.680	1.00 74.26		ŏ
ATOM	2785	CB	PRO		380	22.266	44.567	128.920	1.00 63.37		С
MOTA	2786	CG	PRO		380	21.606		129.236	1.00 58.13		Č
ATOM ATOM	2787 2788	CD N	PRO		380	20.133		129.464 126.590	1.00 65.64		C N
ATOM	2789	CA	ALA		381	20.201		125.348	1.00 66.00	_	Ċ
MOTA	2790	Ċ	ALA		381	18.875	42.977	124.656	1.00 59.33		¢
MOTA	2791	0	ALA		381	17.837		125.292	1.00 53.52		0
ATOM	2792 2793	CB	ALA			20.417 18.952		125.572 123.331	1.00 75.68 1.00 57.68		C N
ATOM ATOM	2794	N CA	CYS		382	17.845		122.410	1.00 60.59		Č
ATOM	2795	c	CYS		382	17.858		121.272	1.00 61.79		č
MOTA	2796	0	CYS		382	18.923		120.747	1.00 58.23		0
ATOM	2797	CB	CYS		382	18.022		121.775	1.00 61.16		c s
ATOM ATOM	2798 2799	SG N	CYS PHE		382 383	16.683 16.704		122.102 120.896	1.00 64.69 1.00 62.44		Ŋ
ATOM	2800	CA	PHE		383	16.664		119.745	1.00 65.46		Ċ
ATOM	2801	С			383	15.710		118.740	1.00 63.82		С
MOTA	2802	0	PHE		383	14.504	41.287	118.950	1.00 61.15		0
ATOM ATOM	2803 2804	CB CG	PHE		383	16.210 16.467		120.105 119.002	1.00 68.56 1.00 76.53		C
ATOM	2805		PHE			17.697		118.339	1.00 74.30		č
ATOM	2806		PHE			15.493	37.281	118.625	1.00 85.67		С
MOTA	2807		PHE			17.948		117.322	1.00 78.20		C
MOTA MOTA	2808 2809	CEZ	PHE			15.741 16.967		117.600 116.956	1.00 88.13 1.00 85.05		C
ATOM	2810	N	ILE			16.270		117.641	1.00 61.06		N
MOTA	2811	CA	ILE			15.488		116.613	1.00 55.74		C
MOTA	2812	C	ILE	Α	384	15.298		115.371	1.00 49.69		¢
MOTA	2813	O CP	ILE			16.260		114.751 116.179	1.00 52.06		0
ATOM ATOM	2814 2815	CB CG1	ILE			16.169 16.669		117.408	1.00 60.45 1.00 57.21		ç
ATOM	2816		ILE			15.218	44.509	115.343	1.00 59.27		С
MOTA	2817	CD1	ILE	Α	384	17.616		117.089	1.00 53.54		C
MOTA	2818	N	THR			14.054		114.993	1.00 42.27		N
ATOM ATOM	2819 2820	CA C	THR THR			13.802 13.050		113.809 112.841	1.00 45.98 1.00 38.79		C
MOTA	2821	ŏ	THR			11.914	41.861	113,113	1.00 41.54		ŏ
MOTA	2822	СВ	THR	Α	385	12.955	39.324	114.165	1.00 48.95		C
MOTA	2823		THR			11.600		114.386	1.00 60.41		0
MOTA MOTA	2824 2825	CG2 N	THR GLN			13.475 13.693		115.460 111.731	1.00 52.69 1.00 34.79		C N
ATOM	2826	CA			386	13.023		110.781	1.00 35.28		Ċ

MOTA	2827	С	GLN	Α	386	11.727	41 981	110.476	1 00	39.22	С
	2828		GLN			11.722					ō
ATOM		0						110.138		40.71	
MOTA	2829	CB	GLN .	Α	386	13.821	42.866	109.499	1.00	34.63	С
MOTA	2830	CG	GLN	Α	386	13.158	43.880	108.566	1.00	34.28	С
MOTA	2831	CD	GLN			14.026		107.386		46.71	Ċ
MOTA	2832		GLN			13.732	43.941	106.249	1.00	48.69	0
ATOM	2833	NE2	GLN .	Α	386	15.093	45.029	107.653	1.00	49.83	N
ATOM	2834	N	LEU			10.616		110.641		43.59	N
MOTA	2835	CA	LEU .			9.322	42.060	110.402	1.00	39.83	С
ATOM	2836	С	LEU .	A	387	8.754	42.574	109.107	1.00	38.85	С
ATOM	2837	Õ	LEU			7.693		108.675		34.66	Ō
MOTA	2838	CB	LEU .			8.361	42.3/5	111.552		33.47	С
MOTA	2839	CG	LEU .	A.	387	7.307	41.314	111.857	1.00	41.41	С
ATOM	2840	CD1	LEU	Δ	3.87	7.998		112.168	1 00	43.33	С
ATOM	2841	CDZ	LEU .		-	6.451		113.042		41.38	С
ATOM	2842	N	LEU .	Α	388	9.478	43.509	108.492	1.00	40.99	N
ATOM	2843	CA	LEU			9.072		107.232	1 00	35.75	С
											č
ATOM	2844	С	LEU			10.209		106.694		35.19	
ATOM	2845	0	LEU	Α	388	10.972	45.589	107.447	1.00	36.99	0
ATOM	2846	CB	LEU .			7.828		107.452	1.00	33.28	С
											č
ATOM	2847	CG	LEU			6.511		106.742		25.74	_
MOTA	2848	CD1	LEU .	Α	388	6.390	43.189	106.470	1.00	38.31	С
MOTA	2849	CD2	LEU .	Α	388	5.361	45.132	107.613	1.00	8.19	С
	2850		PRO			10.282		105.374		28.44	N
MOTA		N									
ATOM	2851	CA	PRO	A	389	9.391		104.403		30.70	С
ATOM	2852	С	PRO	Α	389	9.762	43.081	104.051	1.00	44.42	С
	2853		PRO			9.282		103.049		50.46	0
ATOM		0									č
ATOM	2854	CB	PRO	A	389	9.529		103.206		26.67	C
ATOM ·	2855	CG	PRO	Α	389	11.014	45.718	103.228	1.00	16.13	С
MOTA	2856	CD	PRO			11.281	45 990	104.695	1 00	24.47	С
										47.57	
MOTA	2857	N	VAL			10.583		104.876			Ŋ
ATOM	2858	CA	VAL	Α	390	11.014	41.060	104.559	1.00	49.10	С
ATOM	2859	С	VAL	Δ	390	11.239	40.095	105.724	1.00	51.10	č
											ō
MOTA	2860	0	VAL			11.924		105.595		56.56	
ATOM	2861	CB	VAL	Α	390	12.295	41.094	103.725	1.00	50.36	С
ATOM	2862	CG1	VAL	Α	390	12.050	41.882	102.446	1.00	54.46	С
								104.509		53.00	Ċ
ATOM	2863		VAL			13.413					
ATOM	2864	N	LYS	Α	391	10.669	40.409	106.869	1.00	53.92	N
MOTA	2865	CA	LYS	А	391	10.813	39.520	108.008	1.00	60.85	С
						12.118		107.999		61.60	C
MOTA	2866	С	LYS								
MOTA	2867	0	LYS	Α	391	12.127	37.511	107.688	1.00	60.62	0
ATOM	2868	CB	LYS	А	391	9.621	38.557	108.077	1.00	70.30	С
						9.581		109.393		73.84	Ċ
MOTA	2869	CG	LYS								2
MOTA	2870	CD	LYS	Α	391	8.354	36.840	109.609	1.00	82.47	С
MOTA	2871	CE	LYS	Α	391	8.162	36.436	111.105	1.00	78.17	С
ATOM	2872	NZ				8.786		111.446		72.08	N
			LYS								
MOTA	2873	N	ARG	А	392	13.211		108.350		65.79	. N
ATOM	2874	CA	ARG	Α	392	14.525	38.755	108.408	1.00	66.82	С
MOTA	2875	C	ARG			14.923		109.880	1 00	71.20	С
ATOM	2876	0	ARG	A	392	14.436		110.699		71.14	0
ATOM	2877	ÇВ	ARG	Α	392	15.542	39.599	107.632	1.00	62.17	С
ATOM	2878	CG	ARG			16.666	38.800	106.997	1.00	67.14	С
											č
ATOM	2879	CD	ARG			17.945		106.871		73.94	
ATOM	2880	NE	ARG	Α	392	17.705	40.942	106.318	1.00	76.16	N
ATOM	2881	CZ	ARG	Δ	392	17.244	41.171	105.095	1.00	78.98	С
										83.20	N
ATOM	2882	NH1				16.970		104.285			
ATOM	2883	NH2	ARG			17.056		104.678		79.61	N
ATOM	2884	N	LYS	Α	393	15.826	37.763	110.204	1.00	74.34	N
ATOM	2885	CA	LYS			16.272		111.581	1.00	74.32	С
		Č				17.596		111.894		71.12	č
ATOM	2886		LYS								
ATOM	2887	0	LYS	Α	393	18.653	37.631	111.738		72.31	0
ATOM	2888	CB	LYS			16.400	36.075	111.864	1.00	76.52	C
ATOM	2889	ĊĠ	LYS			15.440		112.894		81.26	С
											č
ATOM	2890	CD	LYS			15.657		113.031		84.21	Č
ATOM	2891	CE	LYS	Α	393	14.564	33.355	113.854		84.12	С
ATOM	2892	NZ	LYS			14.722	31.869	113.887		82.65	N
								112.344		64.44	N
ATOM	2893	N	LEU			17.548					
ATOM	2894	CA	LEU			18.777		112.666		65.62	C
ATOM	2895	С	LEU			19.271	39.597	113.969	1.00	71.87	С
	2896	ŏ	LEU			18.498		114.682		74.80	Ō
ATOM											
ATOM	2897	CB	LEU			18.479		112.818		61.06	C
MOTA	2898	CG	LEU	Α	394	17.758	42.207	111.579	1.00	56.94	С
ATOM	2899		LEU			17.339		111.798		57.94	C
											C C
MOTA	2900		LEU			18.673		110.372		63.83	
ATOM	2901	N	GLY	Α	395	20.548		114.286	1.00	76.02	N
MOTA	2902	CA	GLY			21.085	39.223	115.522	1.00	73.17	С
						20.680		116.826		65.34	č
ATOM	2903	c	GLY								o
MOTA	2904	0	GLY			19.613		116.925		57.67	
MOTA	2905	N	PHE	Α	396	21.540		117.835		63.13	N
MOTA	2906	CA	PHE			21.286	40.392	119.139	1.00	62.22	С
ATOM	2907	c	PHE			21.911		119.160		62.91	č
011	2,01	_	1115	~	550	22.711			1.00	52.71	•

ATOM	2908	0	PHE A	396	22.905	42.023 118.480	1.00 68.68	0
ATOM	2909	СВ	PHE A		21.903	39.557 120.259	1.00 61.44	С
MOTA	2910	CG	PHE A	396	21.194	38.263 120.515	1.00 57.15	С
ATOM	2911	CD1	PHE A	396	20.789	37.923 121.806	1.00 54.82	C
ATOM	2912		PHE A		20.915	37.388 119.472	1.00 59.67	Č
ATOM	2913			396				c c
					20.107	36.725 122.052	1.00 52.15	Č
ATOM	2914	CE2	PHE A	396	20.237	36.190 119.701	1.00 61.55	С
MOTA	2915	CZ	PHE A	396	19.830	35.856 120.991	1.00 58.19	С
ATOM	2916	N	TYR A		21.338	42.689 119.942	1.00 56.31	N
ATOM	2917	CA	TYR A	397	21.862	44.049 120.035		
							1.00 51.12	c
MOTA	2918	С	TYR A		22.132	44.491 121.470	1.00 50.69	С
MOTA	2919	0	TYR A	397	21.259	44.430 122.331	1.00 51.70	0
MOTA	2920	СВ	TYR A	397	20.903	45.036 119.355	1.00 51.25	С
ATOM	2921	CG	TYR A	397	20.898	44.941 117.840	1.00 47.50	Ċ
								ž
MOTA	2922		TYR A		20.283	43.874 117.183	1.00 44.72	C
ATOM	2923	CD2	TYR A	397	21.560	45.891 117.067	1.00 49.23	С
ATOM	2924	CE1	TYR A	397	20.336	43.757 115.801	1.00 47.21	С
ATOM	2925	CE2	TYR A	397	21.620	45.782 115.686	1.00 47.77	С
ATOM	2926	cz	TYR A		21.011	44.715 115.056	1.00 49.51	Ċ
MOTA	2927	ОН	TYR A		21.108	44.600 113.682	1.00 48.37	0
MOTA	2928	N	GLU A	398	23.362	44.923 121.719	1.00 48.51	N
MOTA	2929	CA	GLU A	398	23.760	45.391 123.037	1.00 51.18	С
ATOM	2930	C	GLU A		23.351	46.838 123.202	1.00 49.09	С
							1.00 45.06	ŏ
ATOM	2931	0	GLU A		23.194	47.559 122.216		
MOTA	2932	СВ	GLU A	398	25.272	45.290 123.220	1.00 57.94	С
ATOM	2933	CG	GLU A	398	25.725	44.056 123.957	1.00 71.18	С
ATOM	2934	CD	GLU A		25.354	42.786 123.238	1.00 77.99	С
								ŏ
ATOM	2935		GLU A		25.703	42.676 122.044	1.00 83.73	
MOTA	2936	OE2	GLU A	398	24.727	41.899 123.865	1.00 76.41	0
ATOM	2937	N	TRP A	399	23.191	47.262 124.453	1.00 47.03	N
ATOM	2938	CA	TRP A	399	22.792	48.631 124.750	1.00 50.15	С
ATOM	2939	C	TRP A		23.728	49.619 124.043	1.00 54.33	Ċ
ATOM	2940	0	TRP A		23.350	50.753 123.751	1.00 58.30	0
MOTA	2941	СВ	TRP A	399	22.815	48.849 126.268	1.00 55.61	С
ATOM	2942	CG	TRP A	399	22.007	50.024 126.770	1.00 57.12	С
ATOM	2943		TRP A		20.647	50.184 126.701	1.00 54.16	С
	2944		TRP A		22.511	51.181 127.447	1.00 62.24	č
ATOM								
MOTA	2945	NE1			20.277	51.367 127.296	1.00 56.16	N
ATOM	2946	CE2	TRP A	399	21.401	52.000 127.760	1.00 65.34	С
ATOM	2947	CE3	TRP A	399	23.794	51.606 127.818	1.00 62.19	С
ATOM	2948	CZ2		399	21.536	53.223 128.427	1.00 76.06	С
								č
ATOM	2949	CZ3			23.929	52.823 128.481	1.00 69.98	
ATOM	2950	CH2	TRP A	399	22.803	53.617 128.778	1.00 76.99	С
ATOM	2951	N	THR A	400	24.953	49.186 123.769	1.00 56.41	N
ATOM	2952	CA	THR A		25.902	50.058 123.085	1.00 56.34	С
						49.815 121.583	1.00 59.91	č
ATOM	2953	Ç	THR A		25.811			
MOTA	2954	0	THR A		26.226	50.657 120.791	1.00 64.35	0
ATOM	2955	CB	THR A	400	27.383	49.837 123.553	1.00 54.34	С
ATOM	2956	0G1	THR A	400	27.846	48.544 123.148	1.00 45.99	0
ATOM	2957		THR A		27.494	49.950 125.071	1.00 57.48	С
						48.662 121.199	1.00 58.74	N
ATOM	2958	N	SER A		25.265			
ATOM	2959	CA	SER A	401	25.121	48.327 119.789	1.00 52.36	С
ATOM	2960	С	SER A	401	24.381	49.451 119.082	1.00 46.82	С
ATOM	2961	0	SER A	401	23.467	50.057 119.639	1.00 56.74	0
ATOM	2962	СB	SER A		24.361	47.014 119.617	1.00 53.66	С
						45.930 120.048	1.00 66.24	ŏ
ATOM	2963	OG	SER A		25.156			
MOTA	2964	N	ARG A		24.806	49.737 117.858	1.00 37.82	N
ATOM	2965	CA	ARG A	402	24.212	50.786 117.055	1.00 35.51	С
ATOM	2966	С	ARG A	402	23.541	50.093 115.868	1.00 33.40	С
ATOM	2967	õ	ARG A		24.171	49.301 115.171	1.00 39.64	ō
							1.00 35.13	Č
ATOM	2968	CB	ARG A		25.311	51.744 116.592		Ċ
ATOM	2969	CG	ARG A		24.822	53.137 116.240	1.00 38.74	Č
ATOM	2970	CD	ARG A	402	25.977	54.027 115.780	1.00 46.52	С
ATOM	2971	NE	ARG A	402	25.556	55.298 115.175	1.00 65.72	N
ATOM	2972	CZ	ARG A		24.891	56.272 115.802	1.00 76.44	С
					24.542		1.00 80.92	N
ATOM	2973		ARG A			56.149 117.081		
ATOM	2974		ARG A		24.590	57.389 115.146	1.00 72.87	N
MOTA	2975	N	LEU A	403	22.262	50.379 115.636	1.00 32.46	N
ATOM	2976	CA	LEU A		21.544	49.728 114.538	1.00 39.75	С
ATOM	2977	c	LEU A		21.524	50.458 113.194	1.00 47.84	Ċ
						51.645 113.119	1.00 53.11	ŏ
ATOM	2978	0	LEU A		21.198			Ž
MOTA	2979	СВ	LEU A		20.112	49.414 114.967	1.00 34.32	c
ATOM	2980	CG	LEU A	403	19.110	49.102 113.850	1.00 23.74	C
ATOM	2981		LEU A		19.665	48.111 112.814	1.00 34.79	С
ATOM	2982		LEU A		17.871	48.552 114.512	1.00 16.75	c
ATOM	2983	N	ARG A		21.856	49.734 112.126	1.00 51.96	N
ATOM	2984	CA	ARG A		21.877	50.330 110.801	1.00 61.16	c
ATOM	2985	С	ARG A		21.007	49.571 109.835	1.00 61.63	C
ATOM	2986	0	ARG A	404	20.941	48.345 109.865	1.00 62.38	0
MOTA	2987	CB	ARG A		23.299	50.360 110.262	1.00 77.33	С
ATOM	2988	CG	ARG A		23.395	50.669 108.777	1.00 93.31	Ċ
017	_,,,,							•

	0000	00 100 1 404				_
MOTA	2989	CD ARG A 404	24.842	50.752 108.330	1.00104.56	С
MOTA	2990	NE ARG A 404	24.958	51.122 106.924	1.00108.36	N
ATOM	2991	CZ ARG A 404	26.087	51.518 106.347	1.00110.69	С
MOTA	2992	NH1 ARG A 404	27.207	51.596 107.054	1.00113.17	N
ATOM	2993	NH2 ARG A 404	26.092	51.853 105.065	1.00115.15	N
ATOM	2994	N SER A 405	20.345	50.311 108.960	1.00 65.87	N
ATOM	2995	CA SER A 405	19.487	49.692 107.965	1.00 64.24	С
MOTA	2996	C SER A 405	19.162	50.670 106.840	1.00 59.61	С
	2997	O SER A 405			1.00 58.40	ŏ
ATOM			19.135	51.885 107.051		
MOTA	2998	CB SER A 405	18.202	49.202 108.629	1.00 64.50	С
ATOM	2999	OG SER A 405	17.527	48.275 107.799	1.00 70.73	0
MOTA	3000	N HIS A 406	18.931	50.127 105.647	1.00 53.12	N
MOTA	3001	CA HIS A 406	18.595	50.934 104.481	1.00 46.56	С
MOTA	3002	C HIS A 406	17.068	50.925 104.277	1.00 35.83	С
MOTA	3003	O HIS A 406	16.404	49.910 104.503	1.00 29.57	0
MOTA	3004	CB HIS A 406	19.293	50.392 103.228	1.00 48.87	С
ATOM	3005	CG HIS A 406	20.771	50.232 103.374	1.00 54.29	С
ATOM	3006	ND1 HIS A 406	21.673	50.862 102.543	1.00 45.66	N
MOTA	3007	CD2 HIS A 406	21.505	49.497 104.243	1.00 61.18	С
	3008	CE1 HIS A 406	22.899	50.521 102.894	1.00 56.81	Ċ
MOTA						
MOTA	3009	NE2 HIS A 406	22.825	49.694 103.924	1.00 64.48	N
MOTA	3010	N ILE A 407	16.517	52.055 103.843	1.00 33.33	N
ATOM	3011	CA ILE A 407	15.079	52.185 103.648	1.00 27.22	C C
						č
MOTA	3012	C ILE A 407	14.763	52.762 102.278	1.00 27.16	
ATOM	3013	O ILE A 407	15.310	53.800 101.900	1.00 32.16	0
ATOM	3014	CB ILE A 407	14.498	53.124 104.715	1.00 23.67	C
						ž
MOTA	3015	CG1 ILE A 407	14.838	52.598 106.109	1.00 16.69	Ċ
MOTA	3016	CG2 ILE A 407	12.999	53.262 104.531	1.00 29.79	С
					1.00 26.25	Ċ
MOTA	3017	CD1 ILE A 407	14.805	53.660 107.162		
MOTA	3018	N ASNA 408	13.864	52.105 101.545	1.00 26.02	N
MOTA	3019	CA ASN A 408	13.477	52.564 100.198	1.00 28.35	С
						č
MOTA	3020	C ASN A 408	12.636	53.842 100.237	1.00 25.53	
MOTA	3021	O ASN A 408	11.939	54.105 101.224	1.00 19.57	0
ATOM	3022	CB ASN A 408	12.662	51.492 99.445	1.00 31.03	С
MOTA	3023	CG ASN A 408	13.443	50.213 99.200	1.00 34.57	Č
MOTA	3024	OD1 ASN A 408	14.671	50.232 99.080	1.00 53.90	0
MOTA	3025	ND2 ASN A 408	12.732	49.094 99.099	1.00 23.17	N
ATOM	3026	N PRO A 409	12.695	54.655 99.161	1.00 25.66	N
ATOM	3027	CA PRO A 409	11.926	55.903 99.075	1.00 25.52	С
MOTA	3028	C PRO A 409	10.425	55.646 99.285	1.00 25.11	С
MOTA	3029	O PRO A 409	9.847	54.751 98.667	1.00 19.70	0
ATOM	3030	CB PRO A 409	12.236	56.402 97.661	1.00 26.57	С
ATOM	3031	CG PRO A 409	13.641	55.958 97.458	1.00 30.00	С
MOTA	3032	CD PRO A 409	13.613	54.536 98.012	1.00 27.07	С
ATOM	3033	N THR A 410	9.811	56.438 100.160	1.00 25.25	N
	3034	CA THR A 410	8.389	56.323 100.490	1.00 21.37	С
ATOM						
MOTA	3035	C THR A 410	8.057	54.967 101.118	1.00 24.99	С
ATOM	3036	O THR A 410	6.888	54.650 101.346	1.00 19.45	0
ATOM	3037	CB THR A 410	7.481	56.535 99.248	1.00 11.71	С
MOTA	3038	OG1 THR A 410	7.290	55.293 98.556	1.00 6.84	0
MOTA	3039	CG2 THR A 410	8.111	57.544 98.297	1.00 18.20	С
MOTA	3040	N GLY A 411	9.094	54.176 101.394	1.00 28.42	N
ATOM	3041	CA GLY A 411	8.908	52.870 102.000	1.00 34.59	Ç
MOTA	3042	C GLY A 411	9.056	52.916 103.518	1.00 38.12	С
MOTA	3043	O GLY A 411	9.206	53.994 104.109	1.00 30.75	0
ATOM	3044	N THR A 412	9.017	51.744 104.153	1.00 35.64	N
MOTA	3045	CA THR A 412	9.139	51.650 105.604	1.00 24.91	С
MOTA	3046	C THR A 412	9.714	50.310 106.065	1.00 34.60	С
ATOM	3047				1.00 43.97	ŏ
ATOM	3048	CB THR A 412	7.769	51.824 106.262	1.00 17.00	С
MOTA	3049	OG1 THR A 412	7.159	53.015 105.761	1.00 12.89	0
					1.00 20.31	Ċ
MOTA	3050	CG2 THR A 412	7.904	51.916 107.786		
MOTA	3051	N VAL A 413	10.626	50.348 107.036	1.00 35.58	N
ATOM	3052	CA VAL A 413	11.212	49.132 107.591	1.00 35.35	С
				48.975 109.005	1.00 37.44	č
ATOM	3053	C VAL A 413	10.678			Ž
MOTA	3054	O VAL A 413	10.978	49.774 109.889	1.00 40.54	0
MOTA	3055	CB VAL A 413	12.738	49.194 107.672	1.00 31.35	С
	3056			48.030 108.500	1.00 32.15	Ċ
MOTA		CG1 VAL A 413	13.255			ž
MOTA	3057	CG2 VAL A 413	13.331	49.134 106.285	1.00 38.55	С
MOTA	3058	N LEU A 414	9.876	47.940 109.205	1.00 34.54	N
	3059		9.262	47.657 110.494	1.00 27.00	c
MOTA		CA LEU A 414				~
ATOM	3060	C LEU A 414	10.077	46.645 111.273	1.00 25.79	C
ATOM	3061	O LEU A 414	10.373	45.560 110.761	1.00 25.63	0
ATOM	3062	CB LEU A 414	7.865	47.099 110.270	1.00 25.75	
				46.677 111.528	1.00 26.71	ž
ATOM	3063	CG LEU A 414	7.129			0 0 0
MOTA	3064	CD1 LEU A 414	7.074	47.856 112.492	1.00 25.98	С
ATOM	3065	CD2 LEU A 414	5.732	46.196 111.139	1.00 23.70	С
		-DE DEG V ATA		46.989 112.511	1.00 20.72	
∑/TV∩M		AL E11 + 41C				
ATOM	3066	N LEU A 415	10.418	46 106 112 340		N
MOTA MOTA		N LEU A 415 CA LEU A 415	11.212	46.105 113.349	1.00 25.29	С
ATOM	3066 3067	CA LEU A 415	11.212	46.105 113.349 45.751 114.611		
MOTA MOTA	3066 3067 3068	CA LEU A 415 C LEU A 415	11.212 10.501	46.105 113.349 45.751 114.611	1.00 25.29 1.00 35.11	c c
ATOM	3066 3067	CA LEU A 415	11.212	46.105 113.349	1.00 25.29	С

ATOM	3070	СВ	LEU	A 4	115	12.512	46.774	113.739	1.00	26.14	С
MOTA	3071	CG	LEU			13.445		112.580		35.73	С
MOTA MOTA	3072 3073		LEU			14.630 13.881		113.057 112.002		32.15 31.51	C C
ATOM	3074	N	GLN			10.909		115.199		45.21	N
ATOM	3075	CA	GLN			10.342		116.465		49.37	Ċ
MOTA	3076	С	GLN			11.462		117.400		49.32	С
ATOM	3077	0	GLN			12.252		117.085		54.45	0
ATOM ATOM	3078 3079	CB CG	GLN GLN			9.384 8.851		116.262 117.555		53.69 61.76	c c
ATOM	3080	CD	GLN			7.948		117.342		70.07	č
ATOM	3081	OE1	GLN	A 4	116	6.852		116.827		69.41	ō
ATOM	3082		GLN			8.412		117.716		71.96	N
MOTA MOTA	3083 3084	N CA	LEU			11.530 12.565		118.551 119.532		44.33	N C
MOTA	3085	C	LEU			12.102		120.757		43.96	č
ATOM	3086	0	LEU			11.068	43.702	121.354	1.00	47.68	0
MOTA	3087	CB	LEU			13.193		120.005		28.58	C
ATOM ATOM	3088 3089	CG	LEU			13.889 12.937		118.965 117.871		23.76 23.16	c c
MOTA	3090		LEU			14.412		119.678		37.98	č
MOTA	3091	N	GLU			12.930		121.129		50.78	N
MOTA	3092	CA	GLU			12.740		122.294		56.06	c c
ATOM ATOM	3093 3094	C O	GLU			13.886 15.048		123.273 122.883		52.73 52.36	0
ATOM	3095	СВ	GLU			12.778		121.878		73.81	С
MOTA	3096	CG	GLU			11.697		120.905		81.37	С
MOTA	3097	CD	GLU			10.318		121.434		88.26 88.90	C
ATOM ATOM	3098 3099		GLU GLU			9.485		122.624 120.664		92.72	Ö
ATOM	3100	N	ASN			13.561		124.547		51.08	N
MOTA	3101	CA	ASN			14.575		125.563		62.26	C
ATOM	3102	C	ASN			15.010 14.160		126.204 126.549		72.70 77.62	C O
ATOM ATOM	3103 3104	СВ	ASN			13.983		126.507		61.20	Č
ATOM	3105	CG	ASN	A 4	119	15.024	43.718	127.495	1.00	66.62	С
MOTA	3106		ASN			15.714		128.242		68.87	0
ATOM ATOM	3107 3108	ND2	ASN THR			15.149 16.317		127.426 126.367		72.89 81.68	N N
ATOM	3109	CA	THR			16.818		126.947		90.74	Ċ
ATOM	3110	С	THR	A 4	120	16.281		128.332		04.05	С
ATOM	3111	0	THR			16.454		128.782		10.21	0
ATOM ATOM	3112 3113	CB OG1	THR			18.366 18.869		126.998 125.693		81.03 75.62	C
ATOM	3114		THR			18.886		127.975		77.69	Č
MOTA	3115	N	MET			15.627		128.998		13.95	N
ATOM	3116	CA	MET			15.065 15.982		130.331 131.225		.20.80 .23.07	C
ATOM ATOM	3117 3118	C O	MET			16.695		132.082		23.93	
ATOM	3119	ČВ	MET	A 4	121	13.688	39.024	130.230	1.001	25.37	С
MOTA	3120	CG	MET			13.707		129.761		32.66	
ATOM ATOM	3121 3122	SD CE	MET			13.245 11.455		128.032 128.169		.39.40 .40.66	s C
TER	3123	CE	MET			11.455	37.300	120.109	1.001	.40.00	•
CHAIN	R										
CHAIN		Acom									
1 mar:		Lype	Res		#	<u>X</u>	<u>Y</u>	2	<u>000</u>	B 34	
ATOM ATOM	3124 3125	N CA	LEU		32 32	18.182 19.509	70.054 70.198	66.135 65.474		79.74 75.16	N C
ATOM	3125	C	LEU		32	19.643	69.164	64.364		74.82	٠ ، ،
MOTA	3127	0	LEU	В	32	19.674	67.959	64.622	1.00	74.40	0
ATOM	3128	CB	LEU		32	20.631	70.015	66.499		69.65	C
MOTA MOTA	3129 3130	CG	LEU		32 32	22.052 22.277	70.032 71.300	65.945 65.142		63.79 69.05	C C
MOTA	3131		LEU		32	23.037	69.926	67.088		60.38	č
MOTA	3132	N	ASP	В	33	19.718	69.637	63.127	1.00	75.12	N
MOTA	3133	CA	ASP		33	19.829	68.743	61.980 61.775		77.12 73.83	c c
ATOM ATOM	3134 3135	C O	ASP ASP		33 33	21.250 21.982	68.235 68.735	60.929		79.11	0
MOTA	3136	СВ	ASP	В	33	19.331	69.453	60.719	1.00	84.26	С
MOTA	3137	CG	ASP	В	33	19.411	68.578	59.477		92.75	С
MOTA MOTA	3138 3139		ASP ASP		33 33	20.533 18.348	68.328 68.142	58.990 58.982		96.10 01.06	0
MOTA	3140	N N	ASN		33 34	21.631	67.237	62.565		68.75	N
MOTA	3141	CA	ASN	В	34	22.955	66.629	62.490	1.00	61.95	С
MOTA	3142	С	ASN		34	22.745	65.183	62.084		61.51	c
MOTA MOTA	3143 3144	O CB	ASN ASN		34 34	23.643 23.625	64.354 66.670	62.194 63.860		62.64	0 C
ATOM	3145	CG	ASN		34	22.702	66.183	64.965		60.45	č

N TOOM	3146	001	ACM D	34	21 071	CC 300	64.744	1.00 75.84	•
MOTA			ASN B		21.873	65.300			0
ATOM	3147	ND2	ASN B	34	22.846	66.751	66.159	1.00 52.80	N
MOTA	3148	N	GLY B	35	21.536	64.889	61.624	1.00 59.99	N
ATOM	3149	CA	GLY B	35	21.211		61.222	1.00 56.70	
						63.539			Ç
ATOM	3150	С	GLY B	35	21.134	62.635	62.432	1.00 51.54	С
MOTA	3151	0	GLY B	35	21.241	61.417	62.310	1.00 50.80	0
ATOM	3152	N	LEU B	36	20.965	63.236	63.606	1.00 50.80	N
ATOM	3153	CA	LEU B	36	20.868	62.473	64.841	1.00 53.80	С
ATOM	3154	С	LEU B	36	19.532	62.692	65.510	1.00 55.66	С
								1.00 54.78	
MOTA	3155	0	LEU B	36	18.915	63.752	65.374		0
MOTA	3156	ÇВ	LEU B	36	21.981	62.851	65.817	1.00 55.51	С
MOTA	3157	CG	LEU B	36	23.391	62.428	65.431	1.00 61.24	С
					24.307		66.627	1.00 69.17	č
MOTA	3158		LEU B	36		62.620			
MOTA	3159	CD2	LEU B	36	23.388	60.968	64.995	1.00 64.69	С
MOTA	3160	N	ALA B	37	19.094	61.682	66.249	1.00 55.44	N
				37	17.823	61.773	66.924	1.00 56.47	Ċ
MOTA	3161	CA	ALA B			-			
MOTA	3162	С	ALA B	37	16.770	62.027	65.857	1.00 55.07	C
ATOM	3163	0	ALA B	37	16.046	63.024	65.910	1.00 61.48	0
				37	17.841		67.929	1.00 48.50	Ċ
ATOM	3164	CB	ALA B			62.910			
MOTA	3165	N	ARG B	38	16.715	61.141	64.864	1.00 52.66	N
MOTA	3166	CA	ARG B	38	15.710	61.260	63.818	1.00 54.70	С
							64.402	1.00 53.28	Ċ
ATOM	3167	С	ARG B	38	14.532	60.514			
MOTA	3168	0	ARG B	38	13.529	60.268	63.745	1.00 56.89	0
MOTA	3169	CB	ARG B	38	16.150	60.591	62.511	1.00 60.48	С
								1.00 67.93	Ċ
MOTA	3170	CG	ARG B	38	17.485	61.061	61.940		
MOTA	3171	CD	ARG B	38	17.698	62.565	62.071	1.00 73.20	С
MOTA	3172	NE	ARG B	38	16.750	63.366	61.302	1.00 75.02	N
								1.00 75.84	ċ
MOTA	3173	CZ	ARG B	38	16.732	64.698	61.314		
ATOM	3174	NH1	ARG B	38	17.607	65.368	62.054	1.00 71.97	N
MOTA	3175		ARG B	38	15.847	65.365	60.587	1.00 71.94	N
ATOM	3176	N	THR B	39	14.708	60.145	65.663	1.00 49.27	N
ATOM	3177	CA	THR B	39	13.718	59.444	66.473	1.00 48.97	С
ATOM	3178	Ċ	THR B	39	14.065	59.752	67.930	1.00 45.13	С
									ō
MOTA	3179	0	THR B	39	15.234	59.923	68.281	1.00 41.30	
ATOM	3180	CB	THR B	39	13.784	57.923	66.284	1.00 51.41	С
ATOM	3181	OG1	THR B	39	15.090	57.453	66.642	1.00 53.32	0
								1.00 53.48	Ċ
MOTA	3182		THR B	39	13.491	57.557	64.849		
ATOM	3183	N	PRO B	40	13.052	59.838	68.797	1.00 43.40	N
ATOM	3184	CA	PRO B	40	13.339	60.129	70.203	1.00 44.54	С
									Ċ
MOTA	3185	С	PRO B	40	14.477	59.233	70.712	1.00 42.84	
ATOM	3186	0	PRO B	40	14.403	58.011	70.602	1.00 41.51	0
ATOM	3187	CB	PRO B	40	12.008	59.833	70.884	1.00 43.15	С
									Č
ATOM	3188	CG	PRO B	40	10.994	60.182	69.811	1.00 45.82	Č
MOTA	3189	CD	PRO B	40	11.614	59.597	68.575	1.00 43.19	С
ATOM	3190	N	THR B	41	15.532	59.845	71.246	1.00 39.69	N
									Ċ
ATOM	3191	CA	THR B	41	16.688	59.104	71.762	1.00 34.79	Č
ATOM	3192	С	THR B	41	16.260	58.125	72.854	1.00 34.75	С
ATOM	3193	0	THR B	41	15.420	58.464	73.688	1.00 39.58	0
						60.046	72.405	1.00 29.69	Ċ
MOTA	3194	СB	THR B	41	17.722				Č
MOTA	3195	OG1	THR B	41	17.911	61.195	71.577	1.00 41.03	0
MOTA	3196	CG2	THR B	41	19.049	59.326	72.584	1.00 27.40	С
					16.844	56.926	72.866	1.00 31.56	N
MOTA	3197	N	MET B	42					
MOTA	3198	CA	MET B	42	16.520	55.931	73.890	1.00 30.99	C C
MOTA	3199	С	MET B	42	17.766	55.515	74.667	1.00 25.79	С
ATOM	3200	ŏ	MET B	42	18.777	55.121	74.066	1.00 22.58	0
								1.00 31.64	č
MOTA	3201	СВ	MET B	42	15.900	54.697	73.256		
ATOM	3202	CG	MET B	42	14.675	54.994	72.465	1.00 30.50	С
ATOM	3203	SD	MET B	42	13.927	53.466	71.905	1.00 35.34	S
ATOM	3204	CE	MET B	42	13.193	52.944	73.482	1.00 33.78	С
ATOM	3205	N	GLY B	43	17.683	55.585	75.997	1.00 17.55	N
ATOM	3206	CA	GLY B	43	18.814	55.216	76.821	1.00 10.11	С
ATOM	3207	c	GLY B	43	18.537	55.205	78.314	1.00 20.21	С
							78.740	1.00 26.95	ŏ
MOTA	3208	0	GLY B	43	17.388	55.113			
ATOM	3209	N	TRP B	44	19.607	55.307	79.105	1.00 24.35	N
ATOM	3210	CA	TRP B	44	19.535	55.295	80.562	1.00 21.41	С
							81.108	1.00 19.25	č
ATOM	3211	C	TRP B	44	20.361	56.447			
MOTA	3212	0	TRP B	44	21.407	56.785	80.560	1.00 17.63	0
ATOM	3213	CB	TRP B	44	20.093	53.977	81.089	1.00 16.55	c c
ATOM	3214	CG	TRP B	44	19.981	53.771	82.580	1.00 14.71	r
									č
MOTA	3215		TRP B	44	18.878	53.325	83.271	1.00 24.41	Ç
ATOM	3216	CD2	TRP B	44	21.010	53.979	83.564	1.00 12.56	Ċ
ATOM	3217		TRP B	44	19.159	53.240	84.622	1.00 21.86	N
									c c
MOTA	3218		TRP B	44	20.456	53.637	84.831	1.00 19.49	Č
MOTA	3219	CE3	TRP B	44	22.340	54.421	83.501	1.00 3.31	С
ATOM	3220		TRP B	44	21.192	53.729	86.028	1.00 18.23	С
						54.508		1.00 18.81	č
ATOM	3221		TRP B	44	23.069		84.685		-
MOTA	3222	CH2	TRP B	44	22.491	54.164	85.934	1.00 21.72	С
MOTA	3223	N	LEU B	45	19.891	57.041	82.193	1.00 14.32	N
ATOM	3224	CA	LEU B	45	20.585	58.151	82.800	1.00 12.02	С
									č
ATOM	3225	C	LEU B	45	20.518	57.949	84.298	1.00 11.86	
MOTA	3226	0	LEU B	45	19.446	57.871	84.893	1.00 9.20	0

ATOM	3227	СВ	LEU B	45	19.912	59.452	82.403	1.00 18.50	С
									č
ATOM	3228	CG	LEU B	45	20.723	60.735	82.556	1.00 20.48	Č
MOTA	3229	CD1	LEU B	45	19.788	61.910	82.353	1.00 38.29	С
MOTA	3230	CD2	LEU B	45	21.364	60.820	83.931	1.00 26.67	С
MOTA	3231	N	HIS B	46	21.688	57.888	84.905	1.00 15.42	N
								1.00 17.99	Ċ
MOTA	3232	CA	HIS B	46	21.811	57.646	86.324		
MOTA	3233	С	HIS B	46	21.165	58.639	87.262	1.00 20.83	С
MOTA	3234	0	HIS B	46	20.859	58.283	88.400	1.00 18.34	0
ATOM	3235	СВ	HIS B	46	23.291	57.539	86.687	1.00 20.83	Ċ
				_					
MOTA	3236	CG	HIS B	46	23.894	58.830	87.147	1.00 34.82	C
MOTA	3237	ND1	HIS B	46	23.752	59.300	88.435	1.00 42.63	N
ATOM	3238	CD2	HIS B	46	24.626	59.759	86.488	1.00 36.96	С
ATOM	3239		HIS B	46	24.372		88.550	1.00 44.35	č
						60.461			
ATOM	3240		HIS B	46	24.911	60.763	87.383	1.00 43.02	N
MOTA	3241	N	TRP B	47	20.925	59.867	86.822	1.00 19.71	N
ATOM	3242	CA	TRP B	47	20.398	60.848	87.770	1.00 28.76	С
ATOM	3243	Ċ	TRP B	47	19.337	60.464	88.817	1.00 27.27	Ċ
									Š
MOTA	3244	0_	TRP B	47	19.682	60.183	89.960	1.00 21.13	0
ATOM	3245	CB	TRP B	47	19.935	62.126	87.074	1.00 34.47	С
ATOM	3246	CG	TRP B	47	19.839	63.234	88.093	1.00 44.39	С
ATOM	3247	CD1		47	18.726	63.955	88.437	1.00 50.83	Č
									č
MOTA	3248		TRP B	47	20.883	63.679	88.960	1.00 40.85	
MOTA	3249	NE1	TRP B	47	19.017	64.813	89.469	1.00 53.15	N
MOTA	3250	CE2	TRP B	47	20.334	64.659	89.812	1.00 43.61	С
MOTA	3251	CE3	TRP B	47	22.229	63.334	89.109	1.00 37.21	С
			TRP B		21.089		90.790	1.00 42.53	č
MOTA	3252	CZ2		47		65.307			Č
MOTA	3253	CZ3	TRP B	47	22.977	63.975	90.077	1.00 43.26	Ċ
ATOM	3254	CH2	TRP B	47	22.404	64.948	90.910	1.00 43.64	С
ATOM	3255	N	GLU B	48	18.059	60.456	88.443	1.00 26.18	N
	3256	CA		48	16.992	60.161	89.403	1.00 26.94	c
MOTA			GLU B						
MOTA	3257	С	GLU B	48	17.236	58.982	90.336	1.00 26.40	С
ATOM	3258	0	GLU B	48	16.961	59.074	91.540	1.00 32.83	0
MOTA	3259	CB	GLU B	48	15.644	59.960	88.688	1.00 23.59	С
ATOM	3260	CG	GLU B	48	14.398	60.028	89.619	1.00 21.37	Ċ
									č
ATOM	3261	CD	GLU B	48	14.277	58.855	90.596	1.00 30.24	
MOTA	3262	OE1	GLU B	48	14.155	57.704	90.140	1.00 25.42	0
ATOM	3263	OE2	GLU B	48	14.293	59.078	91.825	1.00 31.90	0
MOTA	3264	N	ARG B	49	17.764	57.886	89.797	1.00 18.46	N
ATOM	3265	ÇA	ARG B	49	17.980	56.690	90.604	1.00 20.46	Ĉ
ATOM	3266	С	ARG B	49	19.190	56.682	91.510	1.00 16.99	Č
ATOM	3267	0	arg b	49	19.225	55.945	92.491	1.00 9.54	0
ATOM	3268	CB	ARG B	49	18.036	55.455	89.702	1.00 27.12	С
ATOM	3269	CG	ARG B	49	18.027	54.142	90.465	1.00 24.47	c
									č
ATOM	3270	CD	ARG B	49	16.855	54.085	91.440	1.00 39.57	
ATOM	3271	NE	ARG B	49	16.607	52.717	91.874	1.00 46.87	N
ATOM	3272	CZ	ARG B	49	17.402	52.033	92.687	1.00 47.11	С
ATOM	3273		ARG B	49	18.500	52.594	93.173	1.00 45.74	N
	3274			49		50.774	92.983	1.00 51.18	N
MOTA			ARG B		17.112				
MOTA	3275	N	PHE B	50	20.175	57.506	91.187	1.00 14.61	N
MOTA	3276	CA	PHE B	50	21.394	57.538	91.973	1.00 21.31	С
MOTA	3277	С	PHE B	50	21.879	58.925	92.369	1.00 31.87	С
ATOM	3278	ō	PHE B	50	22.846	59.062	93.120	1.00 37.81	0
						56.789	91.201	1.00 19.77	č
ATOM	3279	CB	PHE B	50	22.480				-
MOTA	3280	CG	PHE B	50	22.172	55.332	91.017	1.00 26.51	С
ATOM	3281	CD1	PHE B	50	22.492	54.405	92.004	1.00 34.38	С
ATOM	3282		PHE B	50	21.506	54.892	89.884	1.00 18.64	С
MOTA	3283			50	22.144	53.061	91.857	1.00 39.33	Č
								1.00 24.72	č
MOTA	3284		PHE B	50	21.153	53.545	89.726		
ATOM	3285	CZ	PHE B	50	21.472	52.630	90.710	1.00 30.82	С
ATOM	3286	N	MET B	51	21.205	59.950	91.864	1.00 43.78	N
ATOM	3287	CA	MET B	51	21.568	61.325	92.164	1.00 47.32	С
ATOM	3288	_			23.076	61.517	92.228	1.00 48.94	č
		c		51					č
ATOM	3289	0	MET B	51	23.821	60.934	91.447	1.00 46.96	0
ATOM	3290	CB	MET B	51	20.959	61.738	93.488	1.00 43.64	C
MOTA	3291	CG	MET B	51	19.499	61.462	93.581	1.00 36.00	С
ATOM	3292	SD	MET B	51	18.929	62.237	95.051	1.00 43.28	C S C
ATOM	3293	CE	MET B		18.299	63.762	94.379	1.00 50.05	Ċ
				51					N
MOTA	3294	N	CYS B	52	23.517	62.332	93.176	1.00 49.70	N
MOTA	3295	CA	CYS B	52	24.931	62.623	93.338	1.00 54.28	C
MOTA	3296	C	CYS B	52	25.512	61.922	94.552	1.00 56.80	С
ATOM	3297	ŏ	CYS B	52	25.890	62.565	95.530	1.00 53.20	0
MOTA	3298	СB	CYS B	52	25.119	64.124	93.478	1.00 57.48	č
									s
MOTA	3299	SG	CYS B	52	26.853	64.677	93.566	1.00 73.77	
MOTA	3300	N	ASN B	53	25.591	60.600	94.476	1.00 59.82	Ŋ
MOTA	3301	CA	ASN B	53	26.111	59.793	95.571	1.00 60.46	С
MOTA	3302	C	ASN B	53	27.616	59.596	95.445	1.00 58.92	c c
MOTA	3303	ō	ASN B	53	28.094	59.124	94.413	1.00 56.03	ō
							95.571	1.00 63.87	č
MOTA	3304	CB	ASN B	53	25.418	58.441			č
MOTA	3305	CG	ASN B	53	25.860	57.580	96.705	1.00 68.19	C
MOTA	3306	OD1	ASN B	53	27.047	57.317	96.870	1.00 71.70	0
MOTA	3307		ASN B	53	24.909	57.127	97.503	1.00 71.00	N
					_				

ATOM	3308	N	LEU B	54	28.360	59.928 96	6.500	1.00 56.67	ı N
ATOM	3309	CA	LEU B	54	29.819		6.462	1.00 57.08	C
ATOM	3310	Ċ	LEU B	54			7.529	1.00 61.91	
					30.455				
MOTA	3311	0	LEU B	54	31.636		7.426	1.00 60.19	
MOTA	3312	СВ	LEU B	54	30.471	61.180 96	6.546	1.00 51.97	C
ATOM	3313	CG	LEU B	54	30.143	62.191 99	5.451	1.00 51.87	Ċ
ATOM	3314	CD1	LEU B	54	28.706		5.574	1.00 48.76	
ATOM	3315	CD2		54	31.079		5.588	1.00 58.12	
ATOM	3316	N	ASP B	55	29.683		B.549	1.00 70.74	
ATOM	3317	CA	ASP B	55	30.187	57.742 99	9.648	1.00 77.32	. C
ATOM	3318	С	ASP B	55	30.422	56.293 99	9.242	1.00 76.59	
ATOM	3319	ŏ	ASP B	55	29.631		9.579	1.00 78.43	
			ASP B	55					
ATOM	3320	CB			29.201	57.793 100		1.00 88.92	
MOTA	3321	CG	ASP B	55	29.798	57.286 102		1.00 97.30	
MOTA	3322	OD1	ASP B	55	29.064	57.257 103	3.113	1.00103.84	0
MOTA	3323	OD2	ASP B	55	30.995	56.925 102	2.118	1.00 99.30	0
ATOM	3324	N	CYS B	56	31.520		8.535	1.00 73.09	
MOTA	3325	CA	CYS B	56	31.839		8.077	1.00 76.41	
MOTA	3326	C	CYS B	56	32.452		9.204	1.00 78.53	
MOTA	3327	0	CYS B	56	32.976	52.807 98	B.989	1.00 79.36	
ATOM	3328	CB	CYS B	56	32.784	54.789 96	6.879	1.00 82.84	С
MOTA	3329	SG	CYS B	56	32.138	55.971 95	5.651	1.00 97.54	
ATOM	3330	N	GLN B	57	32.383	54.465 100		1.00 82.60	
MOTA	3331	CA	GLN B	57	32.905	53.825 101		1.00 88.03	
MOTA	3332	С	GLN B	57	31.775	53.063 102		1.00 88.25	
MOTA	3333	0	GLN B	57	31.862	51.855 102	2.485	1.00 94.39	
ATOM	3334	CB	GLN B	57	33.456	54.863 102	2.599	1.00 88.55	C
ATOM	3335	CG	GLN B	57	34.574	55.742 102		1.00 99.60	
					35.706	54.944 101			
ATOM	3336	CD	GLN B	57				1.00105.30	
MOTA	3337		GLN B	57	36.355	54.140 102		1.00105.35	
MOTA	3338	NE2	GLN B	57	35.949	55.164 100	0.147	1.00106.68	N N
ATOM	3339	N	GLU B	58	30.704	53.775 102	2.609	1.00 84.13	N
MOTA	3340	CA	GLU B	58	29.565	53.155 103		1.00 85.28	
ATOM	3341	c	GLU B	58	28.336	53.045 102		1.00 86.43	
MOTA	3342	0	GLU B	58	27.279	52.619 102		1.00 94.69	
MOTA	3343	CB	GLU B	58	29.203	53.945 104		1.00 87.78	c c
MOTA	3344	CG	GLU B	58	30.368	54.171 109	5.457	1.00 95.96	i c
MOTA	3345	CD	GLU B	58	30.004	55.072 106	6.615	1.00106.73	
MOTA	3346		GLU B	58	29.694	56 257 106		1.00111.67	
MOTA	3347	OE2		58	30.018	54.595 107		1.00112.58	
MOTA	3348	N	GLU B	59	28.467	53.436 101		1.00 81.94	
MOTA	3349	CA	GLU B	59	27.354	53.340 100	0.183	1.00 81.74	
MOTA	3350	С	GLU B	59	27.941	53.138 98	8796	1.00 77.25	
ATOM	3351	ŏ	GLU B	59	27.760		7.908	1.00 82.71	
ATOM	3352	CB	GLU B	59	26.507	54.611 100		1.00 85.39	C
MOTA	3353	CG	GLU B	59	25.627	54.740 101		1.00101.19	
MOTA	3354	CD	GLU B	59	24.726	53.529 101	1.668	1.00107.93	C
MOTA	3355	OE1	GLU B	59	24.135	53.059 100	0.676	1.00111.69	0
MOTA	3356	OE2		59	24.587	53.050 102		1.00112.86	
MOTA	3357	N	PRO B	60	28.642		8.589	1.00 69.56	
MOTA	3358	CA	PRO B	60	29.279		7.310	1.00 62.09	C
MOTA	3359	С	PRO B	60	28.385	51.308 96	6.134	1.00 55.61	
MOTA	3360	0	PRO B	60	28.760	51.498 94	4.972	1.00 50.15	
ATOM	3361	CB	PRO B	60	30.239	50.574 97	7.694	1.00 64.29	C
ATOM	3362	ĊĞ	PRO B	60	29.434		8.695	1.00 64.33	
			PRO B		28.812		9.546	1.00 63.79	č
MOTA	3363	CD		60					
MOTA	3364	N	ASP B	61	27.212		6.419	1.00 52.52	
MOTA	3365	CA	ASP B	61	26.320		5.344	1.00 55.79	
MOTA	3366	С	ASP B	61	25.635		4.677	1.00 55.83	C
ATOM	3367	0	ASP B	61	25.386	51.505 93	3.481	1.00 52.43	. 0
MOTA	3368	СВ	ASP B	61	25.286		5.870	1.00 63.61	
ATOM	3369	CG	ASP B	61	25.904		6.236	1.00 69.03	
MOTA	3370		ASP B	61	26.211		5.318	1.00 67.01	
ATOM	3371		ASP B	61	26.097		7.443	1.00 71.87	
MOTA	3372	N	SER B	62	25.345		5.445	1.00 61.52	? N
ATOM	3373	CA	SER B	62	24.699	53.783 94	4.900	1.00 62.49	c c
ATOM	3374	C	SER B	62	25.776	54.741 94	4.388	1.00 55.68	
MOTA	3375	ò	SER B	62	25.516		3.592	1.00 54.63	
ATOM	3376	CB	SER B	62	23.880		5.988	1.00 71.33	
MOTA	3377	OG	SER B	62	22.989		6.659	1.00 78.98	
MOTA	3378	N	CYS B	63	26.995		4.860	1.00 47.03	
ATOM	3379	CA	CYS B	63	28.144		4.520	1.00 48.82	? C
MOTA	3380	Č.	CYS B	63	28.362		3.022	1.00 50.6	
					20.302		2.280	1.00 55.82	
ATOM	3381	0	CYS B	63	28.355				
ATOM	3382.	CB	CYS B	63	29.371		5.212	1.00 61.40) <u>c</u>
MOTA	3383	SG	CYS B	63	30.998		4.398	1.00 90.43	
MOTA	3384	N	ILE B	64	28.546	56.726 92	2.585	1.00 45.46	
ATOM	3385	CA	ILE B	64	28.774		1.173	1.00 41.72	? C
MOTA	3386	Ċ	ILE B	64	30.222		0.743	1.00 45.40	
ATOM	3387	ō	ILE B	64	31.114		0.946	1.00 52.5	
ATOM	3388	СВ	ILE B	64	28.458		0.897	1.00 35.88	
A10M	,,,,,	CB	IDC B	04	20.430	JU. JJ 31		1.00 33.80	, (

MOTA	3389	CGI	ILE	R	64	27.000	58.827	91.255	1.00 4	14 28	С
ATOM	3390			В	64	28.729					Č
							58.878	89.439	1.00		Č
MOTA	3391		ILE		64	26.614	60.270	91.062	1.00		
MOTA	3392	N		В	65	30.454	55.573	90.145	1.00 4		Ŋ
MOTA	3393	CA	SER		65	31.801	55.199	89.711	1.00 4		Ç
MOTA	3394	С	SER	В	65	31.795	54.426	88.410	1.00 4	42.46	С
MOTA	3395	0	SER	В	65	30.788	53.821	88.047	1.00 4	42.39	0
ATOM	3396	CB	SER	В	65	32.465	54.307	90.745	1.00 4	46.37	C
ATOM	3397	OG	SER		65	32.080	52.963	90.507	1.00 4		Ō
MOTA	3398	N	GLU		66	32.940	54.420	87.730	1.00 4		N
ATOM	3399	CA	GLU		66	33.075				55.60	č
							53.693	86.474			
ATOM	3400	C	GLU		66	32.698	52.242	86.694	1.00		Ç
ATOM	3401	0	GLU		66	32.176	51.580	85.806	1.00		Ō
ATOM	3402	CB	GLU	В	66	34.509	53.771	85.942	1.00 5	54.09	С
ATOM	3403	CG	GLU	В	66	35.592	53.461	86.970	1.00 6	53.92	С
ATOM	3404	CD	GLU	В	66	36.947	53.196	86.327	1.00 6	69.85	С
ATOM	3405		GLU	В	66	37.090	52.141	85.679	1.00	73.92	0
ATOM	3406	OE2	GLU		66	37.863	54.037	86.454		72.73	Ó
ATOM	3407	N		В	67	32.977	51.737	87.883		59.92	N
ATOM	3408	CA	LYS		67	32.631	50.360	88.180	1.00 6		. <u>c</u>
ATOM	3409	C		В	67	31.130	50.157	87.967	1.00		C
ATOM	3410	0	LYS		67	30.709	49.204	87.311	1.00		0
ATOM	3411	CB	LYS	В	67	33.033	50.023	89.618	1.00	79.48	С
ATOM	3412	CG	LYS	В	67	34.547	50.023	89.847	1.00 9	91.15	С
ATOM	3413	CD	LYS	В	67	34.911	49.554	91.249	1.0010	00.90	С
MOTA	3414	CE	LYS	В	67	36.418	49.369	91.418	1.0010	05.90	С
ATOM	3415	NZ		В	67	36.765	48.894	92.794	1.0010		Ŋ
ATOM	3416	N	LEU		68	30.333	51.079	88.496	1.00 4		N N
	3417	CA	LEU		68	28.881	51.073	88.369	1.00		C
ATOM											Č
MOTA	3418	Ç	LEU		68	28.386	50.985	86.915	1.00 4		c
ATOM	3419	0	LEU		68	27.645	50.090	86.498		35.63	0
ATOM	3420	CB	LEU		68	28.257	52.198	89.113	1.00 5		С
ATOM	3421	CG	LEU	В	68	26.727	52.242	89.171	1.00 4	48.40	С
ATOM	3422	CD1	LEU	В	68	26.210	50.875	89.600	1.00 5	54.14	С
MOTA	3423	CD2	LEU	В	68	26.261	53.348	90.124	1.00 4	45.95	С
MOTA	3424	N	PHE	В	69	28.803	51.973	86.142	1.00 4	40.32	N
ATOM	3425	CA		В	69	28.400	52.057	84.736	1.00 4		C
ATOM	3426	č	PHE		69	28.738	50.779	83.956	1.00 4		č
	3427	ŏ		В		27, 975	50.352	83.076	1.00		ŏ
MOTA			PHE		69						č
MOTA	3428	CB	PHE		69	29.072	53.268	84 . 075	1.00 4		C
MOTA	3429	CG	PHE	В	69	28.452	54.593	84.465	1.00 4		Č
MOTA	3430		PHE		69	27.190	54.948	83.995	1.00 4		С
ATOM	3431	CD2	PHE	В	69	29.124	55.483	85.297	1.00 4	45.13	С
MOTA	3432	CE1	PHE	В	69	26.616	56.165	84.346	1.00 4	48.56	С
MOTA	3433	CE2	PHE	В	69	28.555	56.701	85.651	1.00 4	47.33	С
MOTA	3434	CZ	PHE		69	27.300	57.041	85.174		51.58	Ċ
ATOM	3435	N		В	70	29.887	50.184	84.282		50.28	N
ATOM	3436	CA		В	70	30.337	48.953	83.637	1.00		Ċ
										63.24	č
MOTA	3437	C	MET		70	29.301	47.882	83.903			
ATOM	3438	0	MET		70	28.943	47.106	83.014	1.00 6		0
ATOM	3439	СВ		В	70	31.671	48.482	84.217		52.36	Ç
MOTA	3440	CG	MET	В	70	32.853	49.354	83.895		72.79	С
ATOM	3441	SD	MET	В	70	34.309	48.718	84.728	1.00	76.49	S
ATOM	3442	CE	MET	В	70	34.462	47.114	83.929	1.00	71.92	С
ATOM	3443	N	GLU		71	28.836	47.826	85.144	1.00 6	52.74	N
ATOM	3444	CA	GLU	В	71	27.849	46.836	85.467	1.00 €	60.66	c
ATOM	3445	Ċ	GLU		71	26.661	47.124	84.582		56.18	С
ATOM	3446	ŏ	GLU		71	26.330	46.328	83.704	1.00		ŏ
ATOM	3447	ČВ	GLU		71	27.443	46.922	86.926	1.00		č
				_							_
ATOM	3448	CC	GLU		71	26.921	45.613	87.451	1.00		C
ATOM	3449	CD	GLU		71	26.586	45.694	88.911	1.00		c
ATOM	3450		GLU		71	26.584	44.640	89.578	1.00		0
MOTA	3451	OE2	GLU	В	71	26.322	46.819	89.387	1.00		0
ATOM	3452	N	MET	В	72	26.045	48.283	84.793	1.00 9	52.94	N
ATOM	3453	CA	MET	В	72	24.887	48.669	84.005	1.00 9	55.03	С
ATOM	3454	С	MET	В	72	25.057	48.295	82.545	1.00 5	55.02	С
ATOM	3455	ŏ	MET		72	24.247	47.548	81.993	1.00		Ō
ATOM	3456	СВ	MET		72	24.611	50.171	84.128	1.00		č
ATOM	3457	CG	MET		72	23.672	50.528	85.269	1.00		č
			MET		72	22.168	49.503	85.293	1.00		Š
ATOM	3458	SD							1.00		Č
ATOM	3459	CE	MET		72	21.816	49.419	87.103			
ATOM	3460	N	ALA		73	26.118	48.796	81.924	1.00		N
ATOM	3461	CA	ALA		73	26.368	48.500	80.522	1.00		C
ATOM	3462	С	ALA		73	26.100	47.025	80.244	1.00		C
ATOM	3463	0	ALA		73	25.221	46.680	79.451	1.00		Ō
ATOM	3464	CB	ALA	В	73	27.804	48.849	80.165	1.00		С
ATOM	3465	N	GLU	В	74	26.850	46.168	80.929	1.00		N
ATOM	3466	CA	GLU		74	26.737	44.725	80.779	1.00	60.28	С
ATOM	3467	C	GLU		74	25.282	44.302	80.665	1.00		С
ATOM	3468	ò	GLU		74	24.871	43.688	79.677	1.00		ŏ
ATOM	3469		CLU		74	27 376	44.027	81.985	1.00		č

MOTA MOTA	3470 3471	CG CD	GLU GLU		74 74	28.317 27.645	42.887 41.798	81.627 80.805	1.00 88.79 1.00100.69	C
ATOM	3472		GLU		74	26.753	41.105	81.341	1.00106.44	ŏ
MOTA	3473	OE2	GLU		74	28.006	41.636	79.619	1.00105.25	0
MOTA	3474	N	LEU		75	24.514	44.660	81.690	1.00 51.75	N
ATOM	3475 3476	CA C	LEU		75 75	23.097 22.227	44.333 44.748	81.783 80.600	1.00 50.39 1.00 48.71	C C
ATOM ATOM	3477	ò	LEU		75	21.553	43.911	79.997	1.00 51.38	Ö
ATOM	3478	СВ	LEU		75	22.512	44.939	83.053	1.00 54.68	č
ATOM	3479	CG	LEU		75	22.923	44.280	84.365	1.00 60.00	С
MOTA	3480		LEU		75	24.431	44.293	84.522	1.00 66.87	C
MOTA MOTA	3481 3482	N N	LEU MET		75 76	22.258 22.214	45.017 46.035	85.507 80.278	1.00 65.84 1.00 44.91	N C
ATOM	3483	CA		В	76	21.392	46.500	79.173	1.00 50.42	Ċ
ATOM	3484	C	MET		76	21.421	45.474	78.046	1.00 55.62	С
MOTA	3485	0		В	76	20.414	45.210	77.394	1.00 62.87	0
ATOM	3486	CB	MET		76 76	21.897 21.718	47.858 48.971	78.686 79.703	1.00 41.64 1.00 39.29	c c
ATOM ATOM	3487 3488	CG SD	MET MET		76	22.349	50.547	79.110	1.00 40.97	5
ATOM	3489	CE	MET		76	21.001	50.979	77.992	1.00 38.29	Č
ATOM	3490	N	VAL		77	22.596	44.890	77.852	1.00 56.45	N
MOTA	3491	CA	VAL		77 77	22.826	43.874	76.832	1.00 57.26 1.00 56.69	C C
ATOM ATOM	3492 . 3493	C 0	VAL VAL		77 77	22.219 21.548	42.535 41.859	77.268 76.486	1.00 58.33	o
ATOM	3494	СB	VAL		77	24.347	43.677	76.595	1.00 58.52	С
ATOM	3495		VAL		77	24.577	42.711	75.467	1.00 64.12	c c
ATOM	3496		VAL		77	25.015	45.014	76.305	1.00 62.67	C N
MOTA MOTA	3497 3498	N Ca	SER SER		78 78	22.463 21.979	42.179 40.937	78.530 79.130	1.00 54.01 1.00 54.88	C
ATOM	3499	c.	SER		78	20.480	40.723	79.009	1.00 59.60	č
ATOM	3500	0	SER		78	20.026	39.975	78.148	1.00 63.77	0
ATOM	3501	CB	SER		78	22.357	40.871	80.604	1.00 53.95	c
MOTA MOTA	3502 3503	OG N	SER		78 79	23.759 19.704	40.876 41.361	80.768 79.876	1.00 55.24 1.00 62.46	О N
ATOM	3504	CA	GLU		79	18.256	41.198	79.840	1.00 65.67	С
ATOM	3505	Ċ	GLU		79	17.596	41.854	78.640	1.00 62.34	С
MOTA	3506	0	GLU		79	16.463	42.319	78.706	1.00 57.87	0
ATOM	3507 3508	CB	GLU		79 79	17.621 18.006	41.771	81.109 82.382	1.00 73.87 1.00 77.59	Ċ
ATOM ATOM	3509	CG CD	GLU		79	17.497	39.608	82.407	1.00 75.00	C C
ATOM	3510		GLU		79	16.351	39.378	81.966	1.00 81.09	0
ATOM	3511		GLU		79	18.244	38.719	82.868	1.00 68.80	0
MOTA	3512	N	GLY		80	18.335	41.892	77.546 76.305	1.00 66.49 1.00 70.49	N C
ATOM ATOM	3513 3514	CA C	GLY		80 80	17.823 17.217	42.437 43.824	76.282	1.00 65.38	Ċ
ATOM	3515	ŏ	GLY		80	16.159	44.027	75.676	1.00 63.73	0
MOTA	3516	N	TRP		81	17.873	44.778	76.938	1.00 58.71	N
ATOM	3517	CA	TRP TRP	B B	81	17.391 17.781	46.155 46.751	76.928 75.582	1.00 49.89 1.00 47.71	C C
ATOM ATOM	3518 3519	C 0		В	81 81	16.982	47.408	74.906	1.00 43.13	0
ATOM	3520	СB		В	81	18.031	46.964	78.046	1.00 39.95	c c
MOTA	3521	CG	TRP	В	81	17.513	46.578	79.378	1.00 41.75	c
ATOM	3522	CD1		В	81	18.116	45.766 46.969	80.293 79.947	1.00 49.58 1.00 44.93	c c
MOTA MOTA	3523 3524	NE1	TRP	В	81 81	16.262 17.316	45.629	81.404	1.00 51.02	N
ATOM	3525	CE2		В	81	16.169	46.356	81.217	1.00 47.47	c
ATOM	3526			В	81	15.206	47.775	79.506	1.00 49.30	c c c
ATOM ATOM	3527 3528		TRP TRP		81 81	15.060 14.102	46.527 47.944	82.055 80.340	1.00 51.93 1.00 54.66	C
ATOM	3529		TRP		81	14.039	47.321	81.597	1.00 56.17	č
ATOM	3530	N	LYS		82	19.026	46.503	75.196	1.00 47.14	N
MOTA	3531	CA	LYS		82	19.542	46.992	73.932	1.00 46.37	c c
MOTA	3532 3533	C 0	LYS LYS		82 82	18.597 18.156	46.581 47.412	72.816 72.034	1.00 42.01 1.00 41.69	0
ATOM ATOM	3534	СВ	LYS		82	20.931	46.414	73.687	1.00 54.64	С
ATOM	3535	CG	LYS		82	21.640	46.992	72.484	1.00 57.29	С
MOTA	3536	CD	LYS		82	23.098	46.567	72.483	1.00 68.46	c
ATOM	3537	CE	LYS		82	23.779 23.091	46.955 46.322	71.188 70.027	1.00 77.68 1.00 86.52	C N
MOTA MOTA	3538 3539	NZ N	LYS ASP		82 83	18.274	45.293	72.768	1.00 40.57	N
MOTA	3540	CA	ASP	В	83	17.377	44.734	71.759	1.00 54.12	С
ATOM	3541	C	ASP		83	16.059	45.499	71.646	1.00 58.47	c
MOTA MOTA	3542 3543	O CB	ASP ASP		83 83	15.521 17.064	45.673 43.269	70.554 72.085	1.00 64.42 1.00 62.53	0 C
ATOM	3544	CG	ASP		83	18.301	42.388	72.105	1.00 66.47	С
MOTA	3545	OD1	ASP	В	83	18.214	41.259	72.633	1.00 69.11	0
MOTA	3546		ASP		83	19.355	42.813	71.594 72.782	1.00 67.33 1.00 59.07	O N
MOTA MOTA	3547 3548	N CA	ALA ALA		84 84	15.541 14.275	45.953 46.678	72.805	1.00 57.00	C
ATOM	3549	c	ALA		84	14.391	48.105	72.302	1.00 53.21	С
MOTA	3550	0	ALA		84	13.398	48.697	71.895	1.00 54.97	0

MOTA	3551	CB	ALA	В	84	13.693	46.672	74.208	1.00 64.01	С
ATOM	3552	N	GLY	В	85	15.595	48.664	72.333	1.00 47.70	N
ATOM	3553	CA	GLY		85	15.761	50.021	71.848	1.00 45.23	Ċ
			GLY							č
ATOM	3554	C			85	16.727	50.905	72.611	1.00 45.80	
ATOM	3555	0	GLY		85	17.442	51.704	72.001	1.00 43.19	0
MOTA	3556	N	TYR	В	86	16.746	50.788	73.938	1.00 45.96	N
MOTA	3557	CA	TYR	В	86	17.640	51.608	74.755	1.00 46.92	С
ATOM	3558	С	TYR	В	86	19.037	51.309	74.270	1.00 47.08	č
		ŏ	TYR							ŏ
ATOM	3559				86	19.473	50.164	74.295		_
ATOM	3560	CB	TYR		86	17.479	51.243	76.222	1.00 52.22	0000000
MOTA	3561	ÇG	TYR	В	86	16.042	51.356	76.651	1.00 52.78	С
MOTA	3562	CD1	TYR	В	86	15.501	52.581	77.023	1.00 50.28	С
ATOM	3563		TYR		86	15.201	50.247	76.616	1.00 56.77	С
			TYR		86	14.154	52.697			Č
ATOM	3564							77.351		_
ATOM	3565	CE2	TYR		86	13.852	50.352	76.939	1.00 59.13	Ċ
MOTA	3566	CZ	TYR	В	86	13.336	51.578	77.307	1.00 60.42	С
MOTA	3567	ОН	TYR	В	86	12.008	51.685	77.646	1.00 66.24	0
ATOM	3568	N	GLU		87	19.732	52.338	73.811	1.00 43.55	N
										Ċ
ATOM	3569	CA	GLU		87	21.066	52.147	73.275	1.00 42.08	_
ATOM	3570	С	GLU	В	87	22.058	53.155	73.814	1.00 32.09	С
ATOM	3571	0	GLU	В	87	23.246	53.075	73.542	1.00 31.92	0
ATOM	3572	CB	GLU	В	87	20.988	52.224	71.756	1.00 57.82	С
ATOM	3573	ĊĠ	GLU		87	22.288	52.407	71.031	1.00 79.46	C
										č
ATOM	3574	CD	GLU		87	22.061	52.534	69.540	1.00 94.32	~
ATOM	3575	OEI	GLU	В	87	21.164	53.316	69.146	1.00 93.22	0
MOTA	3576	OE2	GLU	В	87	22.773	51.859	68.764	1.00105.72	0
ATOM	3577	N	TYR		88	21.564	54.095	74.602	1.00 28.08	N
ATOM	3578	CA	TYR		88	22.418	55.120	75.187	1.00 28.39	Ċ
						22.546				č
MOTA	3579	Ç	TYR		88		55.016	76.705	1.00 32.01	_
ATOM	3580	0	TYR	В	88	21.556	55.062	77.431	1.00 40.48	0
MOTA	3581	CB	TYR	В	88	21.884	56.505	74.829	1.00 33.19	С
ATOM	3582	CG	TYR	В	88	22.226	56.962	73.436	1.00 37.55	С
MOTA	3583		TYR		88	23.396	57.683	73.184	1.00 42.68	С
										č
ATOM	3584		TYR		88	21.375	56.693	72.377	1.00 47.22	_
MOTA	3585		TYR	В	88	23.709	58.133	71.914	1.00 43.08	C
MOTA	3586	CE2	TYR	В	88	21.673	57.136	71.092	1.00 51.13	С
MOTA	3587	CZ	TYR	В	88	22.843	57.860	70.864	1.00 42.93	С
ATOM	3588	ОН	TYR		88	23.136	58.323	69.595	1.00 38.53	0
										N
MOTA	3589	N	LEU		89	23.776	54.885	77.183	1.00 27.32	
MOTA	3590	CA	LEU	В	89	24.037	54.794	78.617	1.00 28.99	С
ATOM	3591	С	LEU	В	89	24.711	56.127	78.944	1.00 32.72	С
ATOM	3592	0	LEU	В	89	25.780	56.433	78.406	1.00 22.54	0
MOTA	3593	СB	LEU		89	24.963	53.605	78.879	1.00 29.88	C
									1.00 40.95	č
ATOM	3594	CG	LEU		89	25.375	53.272	80.302		
MOTA	3595	CDI	LEU	В	89	24.159	53.175	81.182	1.00 55.49	C
ATOM	3596	CD2	LEU	В	89	26.140	51.964	80.284	1.00 37.32	C
ATON	3597	N	CYS	В	90	24.090	56.930	79.804	1.00 39.74	N
ATON	3598	ÇA	CYS		90	24.645	58.242	80.108	1.00 43.17	С
							58.599		1.00 46.82	č
ATOM	3599	Ç	CYS		90	24.920		81.545		
ATOM	3600	0	CYS	В	90	24.175	58.230	82.463	1.00 48.55	0
ATOM	3601	CB	CYS	В	90	23.750	59.298	79.503	1.00 43.07	C
ATOM	3602	SG	CYS	В	90	23.343	58.858	77.818	1.00 53.47	S
ATOM	3603	N	ILE		91	26.006	59.348	81.712	1.00 44.38	N
						26.459	59.813	83.012	1.00 33.49	Ċ
ATOM	3604	ÇA	ILE		91					Č
MOTA	3605	С	ILE	В	91	25.927	61.213	83.230	1.00 34.00	C
ATOM	3606	0	ILE	В	91	25.935	62.044	82.316	1.00 42.32	0
MOTA	3607	CB	ILE	В	91	27.984	59.908	83.084	1.00 26.35	С
MOTA	3608		ILE	В	91	28.613	58.593	82.651	1.00 32.38	С
ATOM	3609		ILE		91	28.408	60.256	84.504	1.00 23.86	С
									1.00 37.01	Č
ATOM	3610		ILE		91	30.107	58.652	82.576		
ATOM	3611	N	ASP		92	25.474	61.471	84.447	1.00 29.43	N
MOTA	3612	CA	ASP	В	92	24.952	62.772	84.791	1.00 31.27	С
ATOM	3613	С	ASP		92	25.983	63.421	85.714	1.00 33.43	С
ATOM	3614	Ō	ASP		92	27.079	62.883	85.915	1.00 35.70	0
ATOM	3615	ČВ	ASP		92	23.586	62.616	85.477	1.00 29.94	Č
										č
ATOM	3616	CG	ASP		92	22.875	63.943	85.688	1.00 30.39	č
MOTA	3617		ASP		92	23.111	64.584	86.735	1.00 32.37	0
MOTA	3618	OD2	ASP		92	22.082	64.348	84.806	1.00 18.07	0
ATOM	3619	N	ASP		93	25.626	64.572	86.269	1.00 32.81	N
ATOM	3620	CA	ASP		93	26.496	65.324	87.158	1.00 36.97	С
ATOM	3621	c	ASP		93	27.234	64.452	88.182	1.00 38.38	č
									1.00 34.55	
ATOM	3622	0	ASP		93	26.832	63.311	88.472		0
MOTA	3623	CB	ASP		93	25.674	66.384	87.903	1.00 40.48	C
ATOM	3624	CG	ASP	В	93	26.494	67.609	88.276	1.00 43.57	С
ATOM	3625		ASP		93	27.712	67.466	88.536	1.00 46.43	0
HOTA	3626		ASP		93	25.915	68.718	88.325	1.00 37.49	Ō
MOTA	3627	N			94	28.325	64.999	88.713	1.00 39.48	N
			CYS				64.320	89.739	1.00 42.25	
ATOM	3628	CA	CYS		94	29.107				C
ATOM	3629	C	CYS		94	30.016	63.202	89.254	1.00 42.15	C
MOTA	3630	0	CYS		94	30.416	62.336	90.028	1.00 36.63	0
MOTA	3631	CB	CYS	В	94	28.154	63.822	90.839	1.00 48.72	C

ATOM	3632	SG	CYS	B 94	27.315	65.237	91.653	1.00 73.66	S
ATOM	3633	N	TRP	B 95	30.366	63.237	87.978	1.00 43.99	N
MOTA	3634	CA	TRP	B 95	31.243	62.219	87.420	1.00 50.45	C
MOTA	3635	С	TRP	B 95	32.653	62.796	87.345	1.00 56.13	C
MOTA	3636	0	TRP		33.629	62.062	87.155	1.00 56.63	0
MOTA	3637	CB	TRP		30.811	61.883	86.002	1.00 54.40	C
MOTA	3638	CG	TRP		30.992	63.057	85.087	1.00 59.17	С
MOTA	3639		TRP		30.086	64.036	84 823	1.00 64.81	c
ATOM	3640		TRP		32.181	63.403	84.354	1.00 63.77	C
MOTA	3641		TRP		30.631	64.968	83.963	1.00 67.76	N
MOTA	3642		TRP		31.910	64.596	83.654	1.00 65.92	c
MOTA	3643		TRP		33.440 32.852	62.808	84.205 82.841	1.00 67.47	C
MOTA MOTA	3644 3645		TRP TRP		34.383	65.218 63.430	83.388	1.00 68.21	Ċ
MOTA	3646	CH2			34.075	64.619	82.709	1.00 71.32	Č
MOTA	3647	N	MET		32.738	64.117	87.469	1.00 65.90	й
ATOM	3648	CA	MET		34.003	64.819	87.355	1.00 75.90	ĉ
ATOM	3649	Ċ	MET		34.798	65.081	88.631	1.00 82.19	č
ATOM	3650	õ	MET		34.248	65.254	89.721	1.00 81.85	Ô
MOTA	3651	СВ	MET		33.766	66.140	86.639	1.00 73.16	С
MOTA	3652	CG	MET	B 96	32.586	66.921	87.183	1.00 68.39	c
MOTA	3653	SD	MET	в 96	32.333	68.458	86.294	1.00 71.72	S
MOTA	3654	CE	MET		31.894	67.850	84.646	1.00 55.21	С
MOTA	3655	N	ALA		36.116	65.098	88.475	1.00 84.61	N
MOTA	3656	CA	ALA		37.002	65.377	89.584	1.00 79.26	C
ATOM	3657	C	ALA		36.835	66.871	89.799	1.00 74.19	C
ATOM	3658	0	ALA		36.292	67.569	88.945	1.00 75.52	0 C
MOTA	3659	CB	ALA	-	38.437 37.294	65.050 67.375	89.209 90.948	1.00 81.06	N N
MOTA MOTA	3660 3661	N CA	PRO PRO		37.241	68.777	91.376	1.00 74.89	C
ATOM	3662	C	PRO		37.700	69.889	90.434	1.00 77.18	č
MOTA	3663	ŏ	PRO		37.198	71.004	90.537	1.00 76.09	ŏ
MOTA	3664	ĊВ	PRO		38.034	68.756	92.672	1.00 79.16	č
MOTA	3665	CG	PRO		37.635	67.444	93.247	1.00 74.74	č
ATOM	3666	CD	PRO		37.786	66.527	92.048	1.00 72.46	c
MOTA	3667	N	GLN	B 99	38.659	69.619	89.551	1.00 80.93	N
MOTA	3668	CA	GLN	B 99	39.103	70.651	88.607	1.00 89.74	С
MOTA	3669	C	GLN	B 99	39.982	70.141	87.464	1.00 95.92	С
MOTA	3670	0	GLN		40.448	69.005	87.477	1.00100.48	o o
MOTA	3671	CB	GLN		39.825	71.799	89.327	1.00 87.34	Č
MOTA	3672	CG	GLN		41.174	71.455	89.914	1.00 94.17	C
MOTA	3673	CD	GLN		41.068	70.662	91.191	1.00 97.88	C
ATOM	3674		GLN		40.660	69.502	91.186	1.00100.01	0
MOTA	3675		GLN		41.428	71.292 70.991	92.304 86.472	1.00 95.39 1.00104.87	N N
MOTA	3676	N CA	ARG		40.212	70.616	85.307	1.00104.87	C
MOTA MOTA	3677 3678	C	ARG ARG		41.010 42.387	70.010	85.681	1.00105.78	č
MOTA	3679	ō	ARG		42.724	69.930	86.856	1.00103.10	ŏ
MOTA	3680	СВ	ARG		41.187	71.831	84.390	1.00118.39	č
MOTA	3681	ĊĞ		B 100	39.943	72.698	84.222	1.00121.02	Ċ
MOTA	3682	CD	ARG		38.970	72.146	83.205	1.00120.33	C
MOTA	3683	NE		B 100	37.794	73.002	83.099	1.00118.72	N
MOTA	3684	cz	ARG		36.891	72.915	82.129	1.00119.00	С
MOTA	3685	NH1	ARG	B 100	37.028	72.009	81.172	1.00116.72	N
MOTA	3686	NH2		B 100	35.847	73.729	82.123	1.00120.98	N
MOTA	3687	N		B 101	43.176	69.753	84.662	1.00103.43	N
ATOM	3688	CA		B 101	44.523	69.247	84.863	1.00104.26	C
ATOM	3689	C		B 101	45.527	70.281	84.358	1.00108.42	C 0
ATOM	3690	O CB		B 101	45.144	71.383 67.909	83.974 84.132	1.00106.79 1.00100.77	Č
ATOM ATOM	3691 3692	CG		B 101 B 101	44.712 44.228	67.944	82.687	1.00 92.36	č
MOTA	3693			B 101	44.716	68.791	81.906	1.00 92.02	ŏ
MOTA	3694	OD2		B 101	43.363	67.111	82.327	1.00 82.12	ŏ
ATOM	3695	N		B 102	46.810	69.933	84.371	1.00112.28	N
MOTA	3696	CA		B 102	47.844	70.850	83.904	1.00113.66	С
ATOM	3697	C		B 102	47.454	71.429	82.549	1.00116.11	С
ATOM	3698	Ō		B 102	47.287	72.641	82.419	1.00116.14	0
ATOM	3699	CB	SER	B 102	49.199	70.133	83.804	1.00110.50	c
MOTA	3700	0G		B 102	49.147	69.033	82.911	1.00107.72	0
ATOM	3701	N		B 103	47.301	70.564	81.547	1.00118.95	N
MOTA	3702	CA		B 103	46.914	71.010	80.210	1.00121.20	C
MOTA	3703	Č		B 103	45.749	71.994	80.371	1.00116.49	C
MOTA	3704	0		B 103	45.803	73.122	79.880 79.342	1.00116.10	0 C
MOTA	3705 3706	CB		B 103 B 103	46.494 46.137	69.808 70.133	77.875	1.00132.15	C
MOTA MOTA	3706 3707	CG CD		B 103	47.341	70.133	76.933	1.00144.43	Č
ATOM	3708			B 103	48.046	69.144	76.819	1.00147.01	ŏ
MOTA	3709			B 103	47.575	71.223	76.297	1.00146.67	ŏ
ATOM	3710	N		B 104	44.712	71.570	81.089	1.00110.30	Ň
MOTA	3711	CA		B 104	43.562	72.428	81.309	1.00105.21	Ċ
MOTA	3712	Ċ		B 104	42.230	71.764	81.005	1.00100.85	Ċ

MOTA	3713	0	GLY B	104	41.174	72.328	81.295	1.00 97.39	0
ATOM	3714	N	ARG B	105	42.273	70.567	80.425	1.00 97.66	N
MOTA	3715	CA	ARG B		41.060	69.833	80.080	1.00 96.21	С
ATOM	3716	C	ARG B		40.377	69.316	81.349	1.00 92.31	С
ATOM	3717	ŏ	ARG B		40.800	69.632	82.462	1.00 87.06	0
ATOM	3718	СB	ARG B		41.402	68.669	79.133	1.00102.87	C
ATOM	3719	CG	ARG B		42.377	69.051	78.008	1.00106.88	C
ATOM	3720	CD	ARG B		42.190	68.239	76.722	1.00106.14	Ċ
ATOM	3721	NE	ARG B		42.501	66.820	76.871	1.00104.40	N
ATOM	3722	CZ	ARG B		42.468	65.940	75.873	1.00102.19	Ċ
ATOM	3723		ARG B		42.139	66.333	74.648	1.00100.44	Ň
ATOM	3724		ARG B		42.754	64.664	76.098	1.00 97.55	N
ATOM	3725	N	LEU B		39.320	68.527	81.183	1.00 91.24	N
ATOM	3726	CA	LEU B		38.579	67.979	82.321	1.00 87.88	Ċ
ATOM	3727	c	LEU B		39.041	66.575	82.654	1.00 88.32	č
ATOM	3728	ŏ	LEU B		39.451	65.818	81.777	1.00 91.46	ŏ
MOTA	3729	СВ	LEU B		37.082	67.957	82.012	1.00 84.87	č
MOTA	3730	CG	LEU B		36.466	69.345	81.848	1.00 84.82	č
			LEU B		35.157	69.284	81.088	1.00 89.63	č
ATOM	3731 3732		LEU B		36.277	69.941	83.226	1.00 88.35	č
ATOM	3733		GLN B		38.959	66.227	83.927	1.00 84.82	Ñ
MOTA	3734	N	GLN B		39.377	64.911	84.358	1.00 80.90	Ċ
MOTA		CA C	GLN B		38.419	64.301	85.362	1.00 75.49	č
MOTA	3735 3736	_	GLN B		38.084	64.911	86.383	1.00 69.14	ŏ
MOTA		O CB	GLN B		40.786	64.985	84.941	1.00 87.71	č
MOTA	3737		GLN B		41.100	66.311	85.611	1.00 93.81	č
ATOM	3738	CG					86.126	1.00 94.11	č
ATOM	3739 3740	CD OE1	GLN B		42.523	66.374 65.855	85.495	1.00 95.26	ŏ
ATOM					42.716	67.023	87.271	1.00 95.42	Ň
ATOM	3741		GLN B ALA B		37.973	63.090	85.052	1.00 72.11	N
ATOM	3742	N			37.056	62.378	85.924	1.00 68.89	č
MOTA	3743	CA	ALA B		37.704	62.219	87.288	1.00 62.15	č
ATOM	3744	C	ALA B		38.926	62.221	87.408	1.00 59.29	ŏ
MOTA	3745	0	ALA B		36.733	61.010	85.337	1.00 77.88	č
ATOM	3746	CB	ALA B		36.881	62.088	88.317	1.00 58.74	N
MOTA	3747	Ŋ	ASP B		37.390	61.914	89.664	1.00 63.20	ĉ
MOTA	3748	CA	ASP B		38.417	60.789	89.614	1.00 67.57	č
MOTA	3749	C	ASP B		38.121	59.685	89.162	1.00 66.44	ŏ
MOTA	3750	0			36.250	61.550	90.601	1.00 65.57	č
MOTA	3751	CB	ASP B		36.661	61.581	92.039	1.00 66.50	č
ATOM	3752	CG	ASP B		37.003	62.676	92.529	1.00 65.69	ŏ
MOTA	3753		ASP B				92.671	1.00 67.73	ŏ
MOTA	3754	OD2			36.646 39.640	60.509 61.058	90.083	1.00 07.73	N
MOTA	3755	N	PRO B		40.723	60.074	90.086	1.00 74.11	č
MOTA	3756	CA	PRO B		40.723	58.753	90.758	1.00 75.23	č
MOTA	3757	C	PRO B		40.658	57.678	90.229	1.00 77.28	ŏ
ATOM	3758	0	PRO B		41.846	60.802	90.823	1.00 77.75	č
ATOM	3759	CB CG	PRO B		41.548	62.248	90.574	1.00 73.78	č
ATOM	3760		PRO B		40.061	62.293	90.763	1.00 72.47	č
MOTA	3761	CĐ	PRO B		39.729	58.847	91.919	1.00 76.43	Ñ
MOTA	3762	N	GLN B		39.361	57.673	92.708	1.00 81.74	c c
MOTA	3763	CA	GLN B		38.176	56.860	92.189	1.00 78.82	č
ATOM	3764	C	GLN B		38.253	55.639	92.087	1.00 77.88	ŏ
MOTA MOTA	3765 3766	O CB	GLN B		39.070	58.085	94.155	1.00 90.62	č
MOTA	3767	CG	GLN B		40.177	58.884	94.838	1.00100.25	č
ATOM	3768	CD	GLN B		40.321	60.285	94.277	1.00105.52	č
ATOM	3769		GLN B		39.362	61.057	94.246	1.00108.75	Õ
ATOM	3770		GLN B		41.524	60.622	93.832	1.00107.34	N
ATOM	3771	N			37.072	57.529	91.887	1.00 76.24	N
ATOM	3772	CA	ARG B		35.884	56.840	91.413	1.00 74.45	Ċ
ATOM	3773	c	ARG B		35.926	56.489	89.933	1.00 74.18	С
ATOM	3774	ŏ	ARG B		35.108	55.701	89.452	1.00 69.32	0
ATOM	3775	СВ	ARG B		34.660	57.688	91.713	1.00 71.64	Ċ
ATOM	3776	CG	ARG B		34.638	58.159	93.140	1.00 71.55	Ċ
ATOM	3777	CD	ARG B		33.308	58.787	93.519	1.00 75.99	Ċ
ATOM	3778	NE	ARG B		33.179	60.207	93.185	1.00 73.11	N
ATOM	3779	CZ	ARG B		32.985	60.693	91.962	1.00 71.80	С
MOTA	3780		ARG B		32.900	59.882	90.914	1.00 62.74	N
ATOM	3781		ARG B		32.850	62.000	91.791	1.00 74.87	N
ATOM	3782	N	PHE B		36.873	57.087	89.217	1.00 71.72	N
MOTA	3783	CA	PHE B		37.061	56.831	87.790	1.00 68.98	Ċ
ATOM	3784	c	PHE B		38.549	56.697	87.486	1.00 72.92	č
ATOM	3785	õ	PHE B		39.110	57.476	86.712	1.00 74.24	Õ
ATOM	3786	СВ	PHE B		36.474	57.966	86.948	1.00 57.79	č
MOTA	3787	CG	PHE B		34.970	58.046	86.993	1.00 49.73	С
ATOM	3788		PHE B		34.178	57.101	86.341	1.00 47.07	С
ATOM	3789		PHE B		34.346	59.075	87.688	1.00 45.23	С
ATOM	3790		PHE B		32.791	57.185	86.381	1.00 45.38	С
ATOM	3791		PHE B		32.960	59.164	87.733	1.00 42.04	С
ATOM	3792	CZ	PHE B		32.181	58.214	87.074	1.00 44.56	С
MOTA	3793	N	PRO B		39.207	55.693	88.087	1.00 73.76	N

ATOM	3794	CA	PRO B	114	40.638	55.464	87.873	1.00 73.60	С
MOTA	3795	C		114	41.066	55.394	86.410	1.00 74.91	c
MOTA	3796	0	PRO B		42.135	55.886	86.051	1.00 77.34	0
ATOM	3797	CB	PRO B	114	40.884	54.148	88.601	1.00 71.20	С
MOTA	3798	CG	PRO B	114	39.944	54.241	89.745	1.00 67.92	C
ATOM	3799	CD	PRO B		38.681	54.747	89.087	1.00 71.98	С
ATOM	3800		HIS B		40.236	54.795	85.565	1.00 74.32	N
		N							
MOTA	3801	CA	HIS B		40.592	54.669	84.160	1.00 83.38	Č
MOTA	3802	С	HIS B	115	40.058	55.806	83.284	1.00 88.29	С
ATOM	3803	0	HIS B	115	39.536	55.562	82.193	1.00 93.80	0
ATOM	3804	CB	HIS B	115	40.110	53.314	83.631	1.00 84.54	С
ATOM	3805	CG	HIS B		40.512	52.154	84.492	1.00 85.82	č
	3806					51.916		1.00 85.46	N
MOTA			HIS B		41.818		84.865		
MOTA	3807		HIS B		39.776	51.162	85.049	1.00 86.92	Č
ATOM	3808	CEI	HIS B	115	41.869	50.830	85.614	1.00 84.63	С
ATOM	3809	NE2	HIS B	115	40.644	50.354	85.740	1.00 86.43	N
ATOM	3810	N	GLY B	116	40.211	57.044	83.752	1.00 89.99	N
ATOM	3811	CA	GLY B		39.733	58.184	82.989	1.00 93.41	C
ATOM	3812	Ċ	GLY B		38.393	57.817	82.393	1.00 94.87	č
ATOM	3813	0	GLY B		37.605	57.146	83.043	1.00 97.79	0
ATOM	3814	N	ILE B	117	38.130	58.232	81 . 162	1.00 93.63	N
ATOM	3815	CA	ILE B	117	36.B66	57.899	80.510	1.00 86.58	С
MOTA	3816	С	ILE B	117	37.137	56.944	79.359	1.00 85.63	С
ATOM	3817	ō	ILE B		36.879	55.751	79:464	1.00 84.99	0
ATOM	3818	СВ	ILE B		36.159	59.165	79.968	1.00 81.68	č
ATOM	3819		ILE B		35.758	60.075	81.137	1.00 81.37	c
MOTA	3820	CG2			34.945	58.779	79.133	1.00 76.81	č
MOTA	3821	CD1			34.826	59.437	82.146	1.00 63.59	С
MOTA	3822	N	ARG B	118	37.672	57.489	78.272	1.00 84.43	N
ATOM	3823	CA	ARG B		38.013	56.735	77.076	1.00 90.21	С
MOTA	3824	Ċ	ARG B		37.834	55.219	77.175	1.00 91.62	Ċ
ATOM	3825	ŏ	ARG B		37.005	54.643	76.471	1.00 95.51	ŏ
ATOM	3826	СВ	ARG B		39.455	57.038	76.681	1.00 94.90	c
MOTA	3827	CG	ARG B		39.860	56.372	75.396	1.00109.87	С
MOTA	3828	CD	ARG B	118	38.921	56.792	74.285	1.00123.26	С
MOTA	3829	NE	ARG B	118	39.258	56.170	73.011	1.00139.42	N
MOTA	3830	CZ	ARG B	118	38.651	56.449	71.861	1.00148.72	С
ATOM	3831	NH1	ARG B		37.670	57.343	71.826	1.00154.54	N
						55.839	70.741	1.00155.19	N.
MOTA	3832	NH2			39.025				
MOTA	3833	N	GLN B		38.628	54.583	78.039	1.00 91.20	Ŋ
MOTA	3834	CA	GLN B	119	38.598	53.129	78.246	1.00 87.63	С
MOTA	3835	С	GLN B	119	37.222	52.592	78.539	1.00 84.54	С
ATOM	3836	0	GLN B	119	36.816	51.558	78.004	1.00 84.72	0
ATOM	3837	СB	GLN B		39.511	52.740	79.395	1.00 87.85	Ċ
ATOM	3838	CG	GLN B		40.964	52.985	79.120	1.00 96.11	č
					41.731	53.239	80.387	1.00102.76	č
MOTA	3839	CD	GLN B						
ATOM	3840		GLN B		41.706	52.427	81.314	1.00108.19	0
MOTA	3841	NE 2	GLN B		42.420	54.374	80.442	1.00107.82	N
MOTA	3842	N	LEU B	120	36.523	-53.287	79.425	1.00 81.03	N
ATOM	3843	CA	LEU B	120	35.172	52.909	79.798	1.00 81.16	С
ATOM	3844	С	LEU B	120	34.296	52.969	78.551	1.00 79.11	c
ATOM	3845	ŏ	LEU B		33.442	52.109	78.337	1.00 80.20	Ō
ATOM	3846	СВ	LEU B		34.636	53.870	80.860	1.00 82.48	č
									č
ATOM	3847	CG	LEU B		33.250	53.540	81.410	1.00 82.24	Č
ATOM	3848		LEU B		33.240	52.126	81.954	1.00 88.20	C
ATOM	3849	CD2	LEU B		32.891	54.525	82.493	1.00 86.14	C
ATOM	3850	N	ALA B	121	34.524	53.992	77.731	1.00 74.63	N
ATOM	3851	CA	ALA B	121	33.773	54.175	76.495	1.00 73.56	С
ATOM	3852	C	ALA B		34.026	52.990	75.566	1.00 77.77	С
ATOM	3853	ŏ	ALA B		33.161	52.612	74.778	1.00 75.40	Ō
ATOM	3854	ČВ	ALA B		34.188	55.472	75.821	1.00 67.34	Č
MOTA					35.217	52.405	75.667	1.00 80.26	N
	3855	N	ASN B					1.00 80.28	C
MOTA	3856	CA	ASN B		35.573	51.254	74.848		
ATOM	3857	C	ASN B		34.767	50.051	75.302	1.00 69.74	c
MOTA	3858	0	ASN B	122	34.318	49.246	74.487	1.00 60.92	0
MOTA	3859	CB	ASN B	122	37.058	50.948	74.977	1.00 73.48	С
MOTA	3860	CG	ASN B		37.916	52.101	74.539	1.00 70.43	С
ATOM	3861		ASN B		37.750	52.625	73.440	1.00 66.39	0
MOTA	3862		ASN B		38.840	52.511	75.397	1.00 77.29	N
	3863				34.594	49.926	76.614	1.00 62.16	N .
MOTA		N	TYR B						N
ATOM	3864	CA	TYR B		33.814	48.825	77.163	1.00 60.68	c
MOTA	3865	c	TYR B		32.346	49.059	76.814	1.00 57.45	Ç
MOTA	3866	0	TYR B		31.596	48.121	76.532	1.00 65.68	0
ATOM	3867	CB	TYR B		33.993	48.738	78.685	1.00 62.55	C
MOTA	3868	CG	TYR B		33.158	47.648	79.333	1.00 75.95	С
ATOM	3869		TYR B		32.736	46.533	78.596	1.00 84.78	r
ATOM	3870		TYR B		32.787	47.725	80.678	1.00 76.33	č
ATOM	3871		TYR B		31.959	45.526	79.174		0 0 0 0
		CEI				46.717	81.272	1.00 88.63	c
MOTA	3872		TYR B		32.011			1.00 84.64	Č
MOTA	3873	CZ	TYR B		31.599	45.622	80.512	1.00 90.58	c
MOTA	3874	ОН	TYR B	123	30.823	44.629	81.079	1.00 91.09	0

MOTA	3875	N	VAL B	124	31.945	50.325	76.835	1.00 47.96	N
			VAL B						
MOTA	3876	CA			30.579	50.702	76.495	1.00 40.47	Č
MOTA	3877	C	VAL B		30.385	50.405	75.022	1.00 36.98	C
MOTA	3878	0	VAL B	124	29.422	49.741	74.635	1.00 32.23	0
MOTA	3879	CB	VAL B	124	30.333	52.209	76.725	1.00 41.05	С
ATOM	3880	CG1	VAL B	124	28.959	52.603	76.192	1.00 57.93	С
MOTA	3881		VAL B		30.449	52.535	78.211	1.00 38.22	č
					31.317				
ATOM	3882	N	HIS B			50.904	74.213	1.00 37.79	N
MOTA	3883	CA	HIS B		31.289	50.699	72.770	1.00 44.03	С
MOTA	3884	С	HIS B	125	31.390	49.215	72.427	1.00 49.90	С
MOTA	3885	0	HIS B	125	30.774	48.750	71.466	1.00 49.08	0
ATOM	3886	CB	HIS B	125	32.437	51.468	72.123	1.00 51.70	C
ATOM	3887	CG	HIS B		32.200	52.941	72.049	1.00 58.07	č
			HIS B		31.181			1.00 67.26	N
ATOM	3888					53.488	71.301		
MOTA	3889		HIS B		32.852	53.983	72.617	1.00 54.50	Č
MOTA	3890		HIS B		31.216	54.805	71.410	1.00 63.10	C
MOTA	3891	NE2	HIS B	125	32.221	55.131	72.203	1.00 53.80	N
MOTA	3892	N	SER B	126	32.173	48.488	73.224	1.00 53.77	N
MOTA	3893	CA	SER B	126	32.365	47.058	73.033	1.00 53.79	С
ATOM	3894	Ċ	SER B		31.012	46.368	73.086	1.00 50.23	č
			SER B		30.654		72.177	1.00 48.90	ŏ
ATOM	3895	0				45.625			
ATOM	3896	CB	SER B		33.344	46.506	74.071	1.00 55.88	c
MOTA	3897	OG	SER B		33.593	45.128	73.854	1.00 60.00	0
MOTA	3898	N	LYS B	127	30.259	46.621	74.152	1.00 48.17	N
MOTA	3899	CA	LYS B	127	28.936	46.022	74.326	1.00 43.19	C
ATOM	3900	С	LYS B	127	27.983	46.468	73.215	1.00 41.85	С
ATOM	3901	ō	LYS B		26.850	45.981	73.122	1.00 42.05	Ō
ATOM	3902	СВ	LYS B		28.363	46.395	75.706	1.00 40.95	č
	3903		LYS B		29.061	45.730	76.897	1.00 52.33	č
ATOM		CG							Č
ATOM	3904	CD	LYS B		28.661	44.257	77.061	1.00 62.13	C
ATOM	3905	CE	LYS B		29.138	43.369	75.907	1.00 70.05	С
ATOM	3906	NZ	LYS B		28.684	41.956	76.050	1.00 77.94	N
ATOM	3907	N	GLY B	128	28.455	47.379	72.364	1.00 40.27	N
ATOM	3908	CA	GLY B	128	27.620	47.865	71.280	1.00 40.59	С
ATOM	3909	C	GLY B	128	26.784	49.080	71.644	1.00 40.05	С
ATOM	3910	ō	GLY B		25.936	49.520	70.860	1.00 36.76	Ō
ATOM	3911	N	LEU B		27.022	49.633	72.829	1.00 37.74	Ň
	3912	CA	LEU B		26.267	50.795	73.275	1.00 37.57	Ċ
ATOM									č
ATOM	3913	C	LEU B		26.992	52.101	73.030	1.00 40.12	
ATOM	3914	0	LEU B		28.150	52.119	72.608	1.00 42.48	0
MOTA	3915	CB	LEU B		25.947	50.663	74.752	1.00 39.84	c
ATOM	3916	CG	LEU B		25.336	49.290	75.001	1.00 48.99	C
MOTA	3917	CD1	LEU B	129	25.295	48.994	76.497	1.00 57.24	Ç
MOTA	3918	CD2	LEU B	129	23.953	49.241	74.365	1.00 51.52	c c
MOTA	3919	N	LYS B	130	26.289	53.195	73.296	1.00 42.18	N
MOTA	3920	CA	LYS B	130	26.840	54.526	73.117	1.00 44.52	C C O
ATOM	3921	С	LYS B		26.832	55.227	74.471	1.00 43.45	С
MOTA	3922	ō	LYS B		25.874	55.112	75.241	1.00 45.86	0
ATOM	3923	ĊВ	LYS B		26.014	55.290	72.071	1.00 48.00	Ċ
	3924	ČĞ	LYS B		25.843	54.502	70.758	1.00 57.40	č
ATOM								1.00 60.91	C C
MOTA	3925	CD	LYS B		25.623	55.398	69.539		Č
ATOM	3926	CE	LYS B		25.521	54.589	68.242	1.00 69.51	C
MOTA	3927	NZ	LYS B	130	26.745	53.785	67.943	1.00 75.65	N
ATOM	3928	N	LEU B	131	27.919	55.934	74.763	1.00 38.94	N
ATOM	3929	CA	LEU B	131	28.068	56.641	76.033	1.00 35.19	С
ATOM	3930	С	LEU B	131	27.713	58.119	75.977	1.00 35.30	Č
ATOM	3931	ō	LEU B		27.893	58.783	74.950	1.00 34.57	0
ATOM	3932	ČВ			29.503	56.511	76.545	1.00 34.64	č
ATOM	3933		LEU B		29.895		77.617		č
ATOM	3934		LEU B		29.198	57.191	78.928	1.00 40.68	C
ATOM	3935		LEU B		31.411	57.551	77.794	1.00 40.94	C
ATOM	3936	N	GLY B	132	27.226	58.620	77.110	1.00 32.17	N
MOTA	3937	CA	GLY B		26.850	60.015	77.225	1.00 34.16	С
MOTA	3938	С	GLY B		27.376	60.621	78.511	1.00 32.84	С
ATOM	3939	ō	GLY B		27.355	59.989	79.565	1.00 25.66	0
ATOM	3940	N	ILE B		27.829	61.863	78.433	1.00 32.91	N
ATOM	3941	CA	ILE B		28.370	62.520	79.601	1.00 35.91	Ċ
ATOM	3942	C	ILE B		27.638	63.813	79.908	1.00 36.56	č
ATOM	3942					64.414	79.037	1.00 34.58	ŏ
		0	ILE B		27.031				č
MOTA	3944	CB	ILE B		29.850	62.811	79.386	1.00 38.58	č
ATOM	3945		ILE B		30.493	63.256	80.700	1.00 34.22	<u>c</u>
MOTA	3946		ILE B		30.012	63.829	78.269	1.00 39.58	000
MOTA	3947	CD1	ILE B		30.528	62.165	81.763	1.00 29.09	С
ATOM	3948	N	TYR B		27.715	64.236	81.158	1.00 39.58	N
MOTA	3949	CA	TYR B		27.060	65.449	81.634	1.00 40.75	С
MOTA	3950	С	TYR B	134	28.064	66.602	81.702	1.00 44.66	С
MOTA	3951	0	TYR B		29.239	66.384	81.981	1.00 47.96	0
ATOM	3952	ČВ	TYR B		26.476	65.159	83.021	1.00 42.20	Ċ
ATOM	3953	CG	TYR B		25.949	66.352	83.771	1.00 40.59	Ċ
ATOM	3954		TYR B		24.587	66.497	84.019	1.00 48.82	c 0 c c
ATOM	3955		TYR B		26.816	67.317	84.271	1.00 42.81	Č
							_		_

ATIOM	3956	CEL	TVD	B 134	24.105	67.572	84.754	1.00 54.88	С
MOTA		_							
MOTA	3957	CEZ		B 134	26.349	68.392	85.000	1.00 53.26	C
MOTA	3958	CZ		B 134	24.995	68.517	85.242	1.00 55.73	C
MOTA	3959	ОН		B 134	24.547	69.590	85.983	1.00 63.04	0
MOTA	3960	N		B 135	27.606	67.824	81.450	1.00 50.40	N
MOTA	3961	CA	ALA	B 135	28.483	68.994	81.505	1.00 53.10	С
ATOM	3962	С	ALA	B 135	27.645	70.196	81.863	1.00 50.94	С
ATOM	3963	0	ALA	B 135	26.420	70.109	81.852	1.00 52.75	0
ATOM	3964	СB		B 135	29.150	69.216	80.166	1.00 56.05	č
ATOM	3965	N		B 136	28.286	71.317	82.182	1.00 47.58	Ň
				B 136	27.517	72.514	82.516	1.00 51.44	Ċ.
MOTA	3966	CA				73.772		1.00 50.71	č
ATOM	3967	C		B 136	28.057		81.870		
ATOM	3968	0		B 136	29.253	74.053	81.926	1.00 52.19	0
MOTA	3969	CB		B 136	27.439	72.738	84.023	1.00 53.41	Ç
MOTA	3970	CG	ASP	B 136	26.253	73.613	84.417	1.00 54.28	С
MOTA	3971	OD1	ASP	B 136	26.169	74.774	83.953	1.00 49.26	0
MOTA	3972	OD2	ASP	B 136	25.403	73.128	85.194	1.00 57.23	0
ATOM	3973	N	VAL	B 137	27.140	74.538	81.285	1.00 50.15	N
ATOM	3974	CA		B 137	27.462	75.772	80.570	1.00 53.39	С
ATOM	3975	Ċ		В 137	28.094	76.859	81.424	1.00 57.91	Ċ
ATOM	3976	ŏ		B 137	28.979	77.579	80.958	1.00 56.13	ŏ
	3977			B 137	26.203	76.369	79.905	1.00 50.32	č
ATOM		CB					80.992		č
ATOM	3978			B 137	25.276	76.941		1.00 49.20	
ATOM	3979			B 137	26.602	77.423	78.899	1.00 46.21	C
ATOM	3980	N		B 138	27.636	76.974	82.665	1.00 60.72	N
MOTA	3981	CA		B 138	28.157	77.997	83.548	1.00 68.11	c
ATOM	3982	С		B 138	29.502	77.752	84.198	1.00 75.30	C
MOTA	3983	0	GLY	B 138	30.329	76.994	83.696	1.00 81.96	0
ATOM	3984	N	ASN	B 139	29.737	78.432	85.316	1.00 76.76	N
MOTA	3985	CA	ASN	B 139	30.986	78.263	86.044	1.00 76.95	С
MOTA	3986	C	ASN	B 139	30.985	76.941	86.823	1.00 72.32	С
ATOM	3987	ō		B 139	32.049	76.426	87.180	1.00 69.26	0
ATOM	3988	СВ		B 139	31.247	79.471	86.970	1.00 84.95	Ċ
	3989	CG		B 139	31.905	80.641	86.235	1.00100.73	č
MOTA					32.837	80.436	85.454	1.00103.77	ŏ
ATOM	3990			B 139					N
ATOM	3991			B 139	31.443	81.863	86.494	1.00114.03	
MOTA	3992	N		B 140	29.795	76.375	87.047	1.00 66.89	N
MOTA	3993	CA		B 140	29.666	75.100	87.772	1.00 58.23	C
ATOM	3994	С	LYS	B 140	28.493	74.240	87.305	1.00 52.16	С
ATOM	3995	0	LYS	B 140	27.529	74.744	86.725	1.00 55.77	0
MOTA	3996	CB	LYS	B 140	29.487	75.337	89.270	1.00 53.93	С
MOTA	3997	CG	LYS	B 140	30.731	75.673	90.030	1.00 58.96	С
ATOM	3998	CD		B 140	30.379	75.977	91.473	1.00 62.89	С
ATOM	3999	ĊE	LYS		31.574	76.508	92.230	1.00 72.22	С
ATOM	4000	NZ		B 140	31.204	77.024	93.572	1.00 67.74	N
	4001	N		B 141	28.591	72.936	87.556	1.00 44.73	N
MOTA					27.522	72.003	87.213	1.00 40.60	Ċ
ATOM	4002	CA		B 141				1.00 39.67	č
ATOM	4003	C		B 141	26.572	72.238	88.380		Ö
ATOM	4004	0		B 141	26.978	72.853	89.368	1.00 37.84	
MOTA	4005	CB		B 141	28.009	70.541	87.265	1.00 41.32	c
MOTA	4006			B 141	28.330	70.175	88.621	1.00 33.01	0
MOTA	4007	CG2	THR	B 141	29.252	70.376	86.424	1.00 55.06	С
MOTA	4008	N	CYS	B 142	25.323	71.788	88.293	1.00 44.64	N
MOTA	4009	CA	CYS	B 142	24.431	72.027	89.419	1.00 54.48	C
ATOM	4010	С	CYS	B 142	25.013	71.360	90.654	1.00 55.63	С
ATOM	4011	0	CYS	B 142	24.552	71.590	91.763	1.00 57.67	0
ATOM	4012	ČВ		B 142	23.010	71.502	89.162	1.00 64.07	С
ATOM	4013	ŠG		B 142	22.094	72.315	87.816	1.00 82.05	S
ATOM	4014	N		B 143	26.046	70.546		1.00 60.48	N
ATOM	4015	CA		B 143	26.692	69.843	91.566	1.00 68.18	Ċ.
ATOM	4015	C		B 143	27.738	70.688	92.290	1.00 73.02	č
				B 143	27.992	70.485	93.476	1.00 76.04	ŏ
ATOM	4017	0			21.774	68.574		1.00 76.04	č
MOTA	4018	CB		B 143	27.335		91.060		N
ATOM	4019	N		B 144	28.335	71.638	91.579	1.00 75.69	
ATOM	4020	CA		B 144	29.349	72.483	92.182	1.00 75.17	C
MOTA	4021	C		B 144	30.660	72.221	91.493	1.00 72.42	
MOTA	4022	0		B 144	31.612	72.984	91.612	1.00 81.53	0
MOTA	4023	N		B 145	30.710	71.120	90.763	1.00 66.62	N
MOTA	4024	CA	PHE	B 145	31.918	70.766	90.043	1.00 66.98	Ç
ATOM	4025	С	PHE	B 145	32.186	71.651	88.847	1.00 66.01	С
ATOM	4026	Ō		B 145	31.343	72.446	88.459	1.00 60.69	0
ATOM	4027	ĊВ		B 145	31.835	69.290	89.625	1.00 71.25	С
ATOM	4028	ČĞ		B 145	31.877	68.341	90.769	1.00 77.67	С
ATOM	4029			B 145	33.013	68.230	91.555	1.00 80.29	č
ATOM	4030			B 145	30.762	67.581	91.078	1.00 81.09	č
ATOM	4031			B 145	33.041	67.351	92.626	1.00 83.24	č
						66.704	92.140	1.00 79.03	č
MOTA	4032			B 145	30.781		92.923	1.00 79.03	Ċ
ATOM	4033	CZ		B 145	31.928	66.601	88.281		N
ATOM	4034	N		B 146	33.391	71.547		1.00 66.92	
MOTA	4035	CA		B 146	33.805	72.326	87.116	1.00 72.84	c c
ATOM	4036	С	PKO	B 146	32.679	72.710	86.171	1.00 74.18	U

MOTA	4037	0	PRO	R	146	31.763	71.937	85.950	1 00	79.02	0
ATOM	4038	СB	PRO			34.812		86.450		70.20	č
ATOM	4039	CG	PRO			35.519	71.406			68.37	č
ATOM	4040	CD	PRO				70.851	87.622		70.17	c
	4041	N	GLY			34.427 32.746	70.561	88.640		69.21	N
ATOM	4042	CA	GLY			31.738	73.935	85.668		62.89	C
ATOM	4043	C	GLY			32.109	74.417	84.761		62.01	c
MOTA	4044						74.050	83.344			
MOTA		0	GLY SER			32.238	72.877	83.002		64.67	0
ATOM	4045	N				32.313	75.061	82.513		59.34	N
MOTA	4046	CA	SER			32.684	74.856	81.114		60.60	C
MOTA	4047	c	SER			32.804	76.228	80.474		63.91	c
MOTA	4048	0	SER			33.196	76.349	79.311		60.85	0
MOTA	4049	CB	SER			31.623	74.024	80.391		58.56	C
MOTA	4050	OG.	SER			31.821	72.637	80.589		55.66	0
ATOM	4051	N	PHE			32.480	77.257	81.258		68.09	N
MOTA	4052	CA	PHE			32.538	78.634	80.789		71.36	C
MOTA	4053	C	PHE			33.915	78.948	80.225		71.71	C
ATOM	4054	0_	PHE			34.918	78.815	80.918		68.70	0
MOTA	4055	CB	PHE			32.208	79.591	81.933		74.46	C
MOTA	4056	CG	PHE			32.067	81.011	81.502		80.96	C
MOTA	4057		PHE			31.299	81.327	80.396		83.72	C
MOTA	4058		PHE			32.679	82.034	82.209		83.76	C C
MOTA	4059		PHE			31.148	82.644	79.989		85.06	Ç
MOTA	4060		PHE			32.533	83.359	81.809		81.79	Č
MOTA	4061	CZ	PHE			31.765	83.664	80.703		83.91	C
MOTA	4062	N	GLY			33.957	79.377	78.968		73.51	N
MOTA	4063	CA	GLY			35.227	79.687	78.337		76.77	Ç
ATOM	4064	С	GLY			36.113	78.455	78.280		81.69	Ç
ATOM	4065	0	GLY			37.287	78.509	78.637		87.49	0
ATOM	4066	N	TYR			35.542	77.340	77.840		82.32	N
ATOM	4067	CA	TYR			36.266	76.084	77.740		78.21	Č
ATOM	4068	C	TYR			35.574	75.220	76.698		72.56	Ċ
ATOM	4069	0	TYR	В	151	36.126	74.218	76.234		67.01	0
MOTA	4070	CB	TYR			36.246	75.347	79.079		85.01	С
MOTA	4071	CG	TYR	В	151	37.105	75.933	80.175		89.11	С
MOTA	4072	CD1	TYR	В	151	38.496	75.857	80.116		93.62	
MOTA	4073	CD2	TYR	В	151	36.526	76.511	81.303		91.80	С
MOTA	4074	CE1	TYR	В	151	39.285	76.335	81.160	1.00	97.48	, C
MOTA	4075	CE2	TYR	В	151	37.308	76.991	82.347		95.25	С
MOTA	4076	CZ	TYR	В	151	38.684	76.900	82.270	1.00	97.70	С
MOTA	4077	ОН	TYR	В	151	39.457	77.376	83.301	1.00	95.96	0
MOTA	4078	N	TYR	В	152	34.358	75.623	76.340	1.00	71.16	N
ATOM	4079	CA	TYR	В	152	33.533	74.908	75.365	1.00	69.56	С
ATOM	4080	С	TYR	В	152	34.365	74.161	74.352	1.00	69.71	C C O
MOTA	4081	0	TYR	В	152	34.414	72.933	74.371	1.00	71.60	0
MOTA	4082	CB	TYR	В	152	32.604	75.880	74.639	1.00	68.44	С
MOTA	4083	CG	TYR	В	152	31.750	76.702	75.583	1.00	64.03	С
MOTA	4084		TYR			30.984	76.088	76.580	1.00	64.13	00000000
MOTA	4085		TYR			31.719	78.095	75.494	1.00	62.52	C
ATOM	4086	CE1	TYR	В	152	30.212	76.848	77.469	1.00	70.44	С
MOTA	4087	CE2	TYR	В	152	30.949	78.863	76.375	1.00	66.13	С
MOTA	4088	CZ	TYR	В	152	30.199	78.239	77.361	1.00	66.32	С
MOTA	4089	ОН	TYR	В	152	29.452	79.005	78.239	1.00	52.68	
MOTA	4090	N	ASP	В	153	35.026	74.900	73.471	1.00	70.05	N
MOTA	4091	CA	ASP	В	153	35.860	74.267	72.459	1.00	77.32	c c o
MOTA	4092	С			153	36.745	73.165	73.063	1.00	76.38	С
ATOM	4093	0	ASP	В	153	36.656	72.005	72.654	1.00	80.52	0
ATOM	4094	CB	ASP	В	153	36.724	75.317	71.752	1.00	81.72	С
MOTA	4095	CG	ASP	В	153	35.897	76.312	70.953	1.00	84.14	С
ATOM	4096	OD1	ASP	В	153	35.091	75.877	70.099		75.91	0
MOTA	4097		ASP			36.063	77.530	71.177	1.00	92.08	0
MOTA	4098	N	ILE	В	154	37.590	73.522	74.031		71.17	N
MOTA	4099	CA	ILE			38.461	72.535	74.662	1.00	66.26	С
MOTA	4100	С	ILE	В	154	37.667	71.296	75.040	1.00	62.46	С
ATOM	4101	0	ILE	В	154	37.888	70.204	74.502	1.00	58.97	0
ATOM	4102	CB	ILE	В	154	39.100	73.077	75. 9 33	1.00	68.18	С
MOTA	4103		ILE	В	154	40.058	74.212	75.590	1.00	66.88	С
MOTA	4104		ILE			39.843	71.972	76.639	1.00	65.40	С
MOTA	4105		ILE			40.717	74.829	76.800	1.00	64.67	С
ATOM	4106	N	ASP			36.739	71.475	75.975		60.27	N
ATOM	4107	CA	ASP			35.888	70.384	76.436		61.51	С
ATOM	4108	C	ASP			35.354	69.547	75.265	1.00	56.82	С
ATOM	4109	ō	ASP			35.524	68.328	75.223	1.00	51.29	0
MOTA	4110	СB	ASP			34.724	70.951	77.254		67.35	С
ATOM	4111	CG	ASP			35.190	71.612	78.532		73.00	С
ATOM	4112		ASP			34.337	72.135	79.280		76.43	0
MOTA	4113		ASP			36.417	71.604	78.785		72.06	0
MOTA	4114	N	ALA			34.717	70.206	74.308		56.69	Ŋ
MOTA	4115	CA	ALA			34.183	69.499	73.162		62.83	Ç
MOTA	4116	С	ALA	В	156	35.229	68.523	72.644		66.71	Č
MOTA	4117	0	ALA	В	156	35.047	67.314	72.730	1.00	70.40	0

ATOM	4118	CB	ALA B 150	33.796	70.486	72.072	1.00 70.53	С
ATOM	4119	N	GLN B 15		69.049	72.123	1.00 69.39	N
MOTA	4120	CA	GLN B 15		68.198	71.590	1.00 69.42	Č
MOTA	4121	С	GLN B 15		67.092	72.591	1.00 64.80	С
MOTA	4122	0	GLN B 15	37.807	65.922	72.224	1.00 67.28	0
MOTA	4123	CB	GLN B 15'	38.660	69.011	71.326	1.00 76.41	С
ATOM	4124	CG	GLN B 15		68.627	70.038	1.00 86.50	Ċ
	4125				68.880			
MOTA		CD	GLN B 15			68.826	1.00 89.81	C
MOTA	4126	OE1	GLN B 15		70.023	68.534	1.00 87.85	0
MOTA	4127	NE2	GLN B 15'	38.120	67.813	68.115	1.00 87.49	N
MOTA	4128	N	THR B 158		67.470	73.859	1.00 55.40	N
ATOM	4129	CA	THR B 158		66.502	74.904	1.00 54.68	ĉ
MOTA	4130	C	THR B 150		65.310	74.725	1.00 58.74	C
MOTA	4131	0	THR B 15		64.237	74.305	1.00 62.62	0
MOTA	4132	CB	THR B 158	37.829	67.111	76.297	1.00 50.56	С
ATOM	4133	OG1	THR B 150	38.733	68.206	76.490	1.00 55.92	0
ATOM	4134		THR B 158		66.066	77.378	1.00 46.19	С
ATOM	4135	N	PHE B 159		65.507	75.035	1.00 59.45	N
MOTA	4136	CA	PHE B 15		64.451	74.905	1.00 57.19	C
MOTA	4137	С	PHE B 159		63.760	73.552	1.00 56.03	С
ATOM	4138	0	PHE B 159	34.990	62.531	73.468	1.00 50.18	0
ATOM	4139	CB	PHE B 159	33.407	65.023	74.972	1.00 55.49	С
ATOM	4140	CG	PHE B 159		65.862	76.173	1.00 54.45	Ċ
								č
ATOM	4141		PHE B 159		65.308	77.440	1.00 54.51	<u> </u>
ATOM	4142		PHE B 159		67.212	76.030	1.00 54.14	C
MOTA	4143		PHE B 159		66.087	78.555	1.00 54.81	С
ATOM	4144	CE2	PHE B 159	32:532	68.000	77.134	1.00 54.93	С
ATOM	4145	CZ	PHE B 159		67.439	78.403	1.00 51.81	С
ATOM	4146	N	ALA B 160		64.570	72.495	1.00 58.19	N
					64.071	71.134	1.00 66.53	Č
ATOM	4147	CA	ALA B 160					Č
ATOM	4148	С	ALA B 160		63.050	71.061	1.00 73.96	Ç
ATOM	4149	0	ALA B 160	36.047	62.001	70.425	1.00 80.27	0
ATOM	4150	CB	ALA B 160	35.341	65.224	70.178	1.00 64.98	С
ATOM	4151	N	ASP B 163	37.295	63.372	71.716	1.00 79.36	N
ATOM	4152	CA	ASP B 16		62.491	71.751	1.00 81.74	C
							1.00 79.93	Č
ATOM	4153	C	ASP B 16		61.253	72.563		~
MOTA	4154	0	ASP B 163		60.122	72.099	1.00 76.06	0
MOTA	4155	CB	ASP B 16	39.643	63.206	72.377	1.00 87.77	С
MOTA	4156	CG	ASP B 163	40.587	63.762	71.340	1.00 94.92	С
MOTA	4157		ASP B 16		64.578	70.501	1.00 97.76	0
ATOM			ASP B 16		63.375	71.362	1.00101.23	ō
	4158							
MOTA	4159	N	TRP B 163		61.490	73.778	1.00 78.90	N
ATOM	4160	CA	TRP B 163	37.286	60.435	74.718	1.00 77.64	С
ATOM	4161	С	TRP B 163	36.407	59.352	74.117	1.00 76.70	С
ATOM	4162	0	TRP B 163	36.345	58.234	74.634	1.00 74.99	0
ATOM	4163	ČВ	TRP B 16		61.043	75.924	1.00 80.13	c
						76.849		č
MOTA	4164	CG	TRP B 16:		61.751		1.00 85.52	_
ATOM	4165		TRP B 163		61.892	76.726	1.00 88.24	Č
MOTA	4166	CD2	TRP B 163	2 37.142	62.371	78.081	1.00 84.79	С
ATOM	4167	NE1	TRP B 163	39.360	62.559	77.813	1.00 87.19	N
ATOM	4168		TRP B 163		62.865	78.662	1.00 82.08	C
ATOM	4169	CE3			62.555	78.754	1.00 87.25	Ċ
							1.00 77.70	č
ATOM	4170		TRP B 16		63.535	79.887		Č
ATOM	4171	CZ3	TRP B 163		63.220	79.971	1.00 88.61	C
MOTA	4172	CH2	TRP B 163	37.142	63.702	80.526	1.00 80.08	С
MOTA	4173	N	GLY B 163	35.728	59.699	73.027	1.00 75.99	N
MOTA	4174	CA	GLY B 16		58.762	72.350	1.00 72.23	С
ATOM	4175	c	GLY B 16		58.855	72.810	1.00 67.68	Ċ
	4176	ŏ	GLY B 16		57.844	72.893	1.00 71.72	ō
ATOM				32.709				
MOTA	4177	N	VAL B 16		60.068	73.110	1.00 59.84	N
ATOM	4178	CA	VAL B 16		60.280	73.571	1.00 54.18	Č
ATOM	4179	С	VAL B 16	30.579	60.240	72.426	1.00 56.41	С
ATOM	4180	Ó	VAL B 16		60.513	71.265	1.00 61.84	0
ATOM	4181	СB	VAL B 16		61.630	74.278	1.00 52.19	С
	4182		VAL B 16		61.743	74.869	1.00 54.51	Ċ
ATOM					61 775	75.357	1.00 57.52	č
ATOM	4183		VAL B 164		61.775			
ATOM	4184	N	ASP B 16		59.898	72.760	1.00 56.55	N
ATOM	4185	CA	ASP B 16		59.829	71.756	1.00 56.28	C
ATOM	4186	С	ASP B 16	5 27.177	60.794	72.079	1.00 52.94	С
ATOM	4187	O	ASP B 16		61.164	71.197	1.00 55.38	0
ATOM	4188	СВ	ASP B 16		58.419	71.677	1.00 54.55	Ċ
	4189		ASP B 16		57.377	71.360	1.00 59.13	č
MOTA		CG				70.301		ŏ
ATOM	4190		ASP B 16		57.484		1.00 64.14	
ATOM	4191		ASP B 16		56.448	72.179	1.00 62.71	0
MOTA	4192	N	LEU B 16	27.082	61.211	73.335	1.00 41.96	N
MOTA	4193	CA	LEU B 16		62.115	73.726	1.00 34.65	С
MOTA	4194	c	LEU B 16		63.017	74.896	1.00 36.39	Ċ
MOTA	4195	ŏ	LEU B 16		62.579	75.853	1.00 34.13	ŏ
					61.288	74.067		č
ATOM	4196	CB	LEU B 16				1.00 36.44	c c
ATOM	4197	CG	LEU B 16		61.955	74.604	1.00 40.91	Č
ATOM	4198	CD1	LEU B 16	5 22.372	60.921	74.633	1.00 48.27	С

									•
MOTA	4199	CD2	LEU	В 166	23.718	62.530	75.999	1.00 39.68	С
MOTA	4200	N		B 167	25.939	64.275	74.822	1.00 38.87	N
	4201	CA		B 167	26.211	65.256	75.878	1.00 37.54	ċ
MOTA	4202	c		B 167	24.970	65.902	76.508	1.00 39.34	č
MOTA	4203	ŏ		B 167	24.131	66.474	75.812	1.00 34.28	ŏ
ATOM	4204	СВ		B 167	27.103	66.383	75.339	1.00 39.21	č
ATOM		CG		B 167	27.327	67.493	76.372	1.00 43.73	č
MOTA	4205		LEU		28.163	66.910	77.477	1.00 38.20	č
MOTA	4206						75.769	1.00 43.30	č
MOTA	4207		LEU !		28.017 24.854	68.711 65.815	77.824	1.00 45.42	N
MOTA	4208	N		B 168					Č
MOTA	4209	CA		B 168	23.739	66.459	78.502	1.00 47.97	Ċ
MOTA	4210	C		B 168	24.297	67.786	78.993	1.00 48.67	
MOTA	4211	0		B 168	25.029	67.840	79.994	1.00 53.51	0
MOTA	4212	CB		B 168	23.238	65.632	79.701	1.00 58.69	C C
MOTA	4213	CG		B 168	22.174	66.356	80.567 81.651	1.00 49.99	c
MOTA	4214	CD		B 168	21.531	65.474		1.00 49.99	c
ATOM	4215	CE		B 168	20.366	66.183	82.344	1.00 40.97	N
MOTA	4216	NZ		B 168	19.583	65.271	83.228	1.00 45.83	
MOTA	4217	N		B 169	23.968	68.860	78.292		N C
ATOM	4218	CA		B 169	24.479	70.154	78.703	1.00 51.92	c
MOTA	4219	C		B 169	23.537	70.897	79.656	1.00 51.04 1.00 52.94	0
MOTA	4220	0		B 169	22.569	71.531	79.238	1.00 52.94	
MOTA	4221	CB		B 169	24.779	70.998	77.470		c c c c
MOTA	4222	CG		B 169	25.913	71.948	77.665	1.00 70.42 1.00 72.62	Č
MOTA	4223			B 169	27.112	71.500 73.286	78.199 77.319	1.00 72.82	Č
ATOM	4224			B 169	25.786			1.00 74.80	Č
ATOM	4225			B 169	28.168	72.369	78.388		Č
MOTA	4226			B 169	26.837	74.165	77.504	1.00 74.97 1.00 78.45	Ċ
ATOM	4227	CZ		B 169	28.033	73.706	78.040		N
ATOM	4228	N		B 170	23.834	70.801	80.946	1.00 49.60	C
ATOM	4229	CA		B 170	23.043	71.440	81.989	1.00 48.02	
ATOM	4230	Ç		B 170	23.400	72.925	82.095	1.00 47.03	C
ATOM	4231	0		B 170	24.450	73.344	81.642	1.00 44.69	0
ATOM	4232	CB		B 170	23.313	70.723	83.315	1.00 50.49	C
MOTA	4233	CG		B 170	22.397	71.171	84.424	1.00 53.05	C
MOTA	4234			B 170	21.655	72.153	84.243	1.00 51.74	0
MOTA	4235			B 170	22.421	70.538	85.493	1.00 55.89	0
MOTA	4236	N		B 171	22.529	73.720	82.702	1.00 48.16	N
ATOM	4237	CA		B 171	22.803	75.142	82.827	1.00 52.27	C
MOTA	4238	C		B 171	22.651	75.797	84.196	1.00 51.81	C
ATOM	4239	0		B 171	21.801	76.667	84.401	1.00 48.95	0
MOTA	4240	N		B 172	23.486	75.393	85.141	1.00 56.08	N
ATOM	4241	CA		B 172	23.446	75.986	86.467	1.00 59.63	C
ATOM	4242	С		B 172	24.604	76.961	86.546	1.00 65.06	C
ATOM	4243	0		B 172	25.689	76.671	86.041	1.00 65.52	0
MOTA	4244	CB		B 172	23.627	74.920	87.551	1.00 62.77	c
MOTA	4245	SG		B 172	22.108	74.277	88.318	1.00 73.86	S
MOTA	4246	N		B 173	24.374	78.119	87.154	1.00 69.24	N
MOTA	4247	CA		B 173	25.440	79.102	87.330	1.00 72.13	c
MOTA	4248	С		B 173	25.908	79.893	86.103	1.00 78.33	C
MOTA	4249	0		B 173	26.773	79.439	85.358	1.00 79.20	0
MOTA	4250	CB		B 173	26.674	78.422	87.944	1.00 68.03	C
MOTA	4251	CG		B 173	26.424	77.709	89.252	1.00 71.50	C
ATOM	4252			B 173	25.960	78.405	90.367	1.00 73.51	C
ATOM	4253			B 173	26.663	76.345	89.380	1.00 72.27	c
MOTA	4254			B 173	25.740	77.763	91.586	1.00 70.46	c
MOTA	4255			B 173	26.450	75.687	90.593	1.00 70.67 1.00 66.70	C C
ATOM	4256	CZ		B 173	25.985	76.404	91.695		Ö
ATOM	4257	ОН		B 173	25.752 25.351	75.776		1.00 51.73 1.00 85.92	N
ATOM	4258	N		B 174		81.083	85.911		C
ATOM	4259	CA		B 174	25.755	81.959	84.810	1.00 97.17	Ċ
ATOM	4260	Č		B 174	25.051	83.306	84.934	1.00106.31	0
ATOM	4261	0		B 174	23.869	83.370	85.273	1.00100.13	c
ATOM	4262	CB		B 174	25.454	81.314	83.455	1.00 93.86	
ATOM	4263	SG		B 174	23.775	80.749	83.264	1.00 93.51	S N
ATOM	4264	N		B 175	25.797	84.378	84.668	1.00116.19	
ATOM	4265	CA		B 175	25.282	85.746	84.761	1.00119.63	C
MOTA	4266	C		B 175	23.905	85.952	84.109	1.00118.97	c
ATOM	4267	0		B 175	22.871	85.756	84.752	1.00116.40	0 C
ATOM	4268	CB		B 175	26.291	86.742	84.157 85.071	1.00119.42	Ċ
MOTA	4269	CG		B 175	27.492	87.015		1.00119.29	0
ATOM	4270			B 175	27.288	87.476	86.216	1.00115.50	
ATOM	4271			B 175	28.644	86.783	84.639	1.00117.38	O N
MOTA	4272	N		B 176	23.888	86.352	82.839	1.00119.54	С И
MOTA	4273	CA		B 176	22.627	86.585 85.648	82.138	1.00115.27	Ċ
MOTA	4274	C		B 176	22.452		80.949		0
ATOM	4275	0		B 176	23.407	84.986	80.530	1.00109.69	c
MOTA	4276	CB		B 176	22.560	88.028	81.652 80.644	1.00117.63	Ö
ATOM	4277	OG		B 176	23.527	88.260 85.593	80.404	1.00114.24	N
ATOM	4278	N		B 177	21.234	84.721	79.261	1.00108.85	C
ATOM	4279	CA	LEU	B 177	20.963	04.741	,,,,	1.00112.78	

ATOM	4280	С	LEU B	177	22.028	84.932	78.207	1.00114.90	С
ATOM	4281	0	LEU B		22.311	84.040	77.415	1.00114.82	0
MOTA	4282	CB	LEU B	177	19.586	84.996	78.653	1.00110.84	C
ATOM	4283	CG	LEU B	177	18.355	84.698	79.523	1.00110.75	С
			LEU B						č
MOTA	4284				17.804	86.036	80.112	1.00112.77	Č
MOTA	4285	CD2	LEU B		17.284	83.868	78.675	1.00107.44	С
MOTA	4286	N	GLU B	178	22.615	86.123	78.194	1.00118.09	N
ATOM	4287	CA	GLU B		23.688	86.406	77.253	1.00125.35	Ĉ
									_
MOTA	4288	С	GLU B	178	24.656	85.232	77.393	1.00119.59	С
MOTA	4289	0	GLU B	178	24.777	84.407	76.489	1.00121.69	0
	4290	ĊВ	GLU B		24.391	87.728	77.608	1.00138.64	Č
MOTA									<u> </u>
MOTA	4291	CG	GLU B	178	23.571	88.994	77.331	1.00149.49	С
MOTA	4292	CD	GLU B	178	23.392	89.265	75.843	1.00156.28	С
ATOM	4293		GLU B		24.415	89.444	75.149	1.00156.37	ō
MOTA	4294	OE 2	GLU B		22.235	89.302	75.365	1.00157.99	0
MOTA	4295	N	ASN B	179	25.307	85.133	78.548	1.00109.35	N
ATOM	4296	CA	ASN B		26.246	84.044	78.782	1.00 97.15	С
MOTA	4297	С	ASN B		25.603	82.693	78.512	1.00 92.68	Ç
MOTA	4298	0	ASN B	179	26.241	81.798	77.950	1.00 93.11	0
ATOM	4299	CB	ASN B	179	26.768	84.102	80.209	1.00 92.23	С
			ASN B						č
MOTA	4300	CG			27.451	85.412	80.512	1.00 91.53	
MOTA	4301	OD1	ASN B	179	28.014	86.049	79.625	1.00 82.19	0
ATOM	4302	ND2	ASN B	179	27.423	85.816	81.770	1.00 96.60	N
ATOM	4303	N	LEU B		24.334	82.556	78.890	1.00 83.99	N
MOTA	4304	CA	LEU B		23.602	81.305	78.683	1.00 75.33	C
MOTA	4305	С	LEU B	180	23.391	80.998	77.197	1.00 70.94	С
ATOM	4306	ō	LEU B		24.110	80.183	76.612	1.00 72.94	Ō
MOTA	4307	CB	LEU B		22.243	81.359	79.401	1.00 72.39	Ċ
MOTA	4308	CG	LEU B	180	21.329	80.129	79.303	1.00 71.48	Č
MOTA	4309	CDI	LEU B	180	22.003	78.938	79.950	1.00 70.99	С
	4310		LEU B		19.996	80.406	79.983	1.00 61.21	Č
MOTA									
MOTA	4311	N	ALA B	181	22.403	81.654	76.597	1.00 66.42	N
MOTA	4312	CA	ALA B	181	22.092	81.447	75.192	1.00 69.48	С
MOTA	4313	C	ALA B		23.353	81.213	74.369	1.00 72.08	С
MOTA	4314	0	ALA B		23.451	80.217	73.650	1.00 69.52	0
MOTA	4315	CB	ALA B	181	21.325	82.644	74.648	1.00 69.42	С
MOTA	4316	N	ASP B	182	24.316	82.127	74.479	1.00 73.10	N
			ASP B		25.567	82.008	73.729	1.00 74.22	Ċ
ATOM	4317	CA							
MOTA	4318	С	ASP B	182	26.276	80.696	74.026	1.00 71.67	С
MOTA	4319	0	ASP B	182	26.692	79.986	73.102	1.00 71.12	0
ATOM	4320	СВ	ASP B		26.515	83.176	74.040	1.00 79.33	C
MOTA	4321	CG	ASP B	182	26.210	84.422	73.213	1.00 87.03	С
MOTA	4322	OD1	ASP B	182	26.068	84.300	71.976	1.00 89.64	0
MOTA	4323		ASP B		26.128	85.526	73.797	1.00 92.53	0
MOTA	4324	N	GLY B	183	26.415	80.387	75.316	1.00 65.63	N
MOTA	4325	CA	GLY B	183	27.071	79.157	75.725	1.00 61.42	С
MOTA	4326	С	GLY B	183	26.472	77.931	75.056	1.00 59.22	С
							74.463	1.00 52.20	ŏ
MOTA	4327	0	GLY B		27.194	77.119			
MOTA	4328	N	TYR B	184	25.153	77.783	75.158	1.00 57.41	N
ATOM	4329	CA	TYR B	184	24.482	76.652	74.534	1.00 54.34	С
ATOM	4330	C	TYR B		24.820	76.682	73.058	1.00 57.82	С
MOTA	4331	0	TYR B		25.421	75.735	72.542	1.00 61.15	0
MOTA	4332	CB	TYR B	184	22.963	76.731	74.734	1.00 46.84	С
ATOM	4333	CG	TYR B	184	22.474	75.982	75.960	1.00 44.73	С
ATOM	4334		TYR B		22.541	74.592	76.023	1.00 45.99	0000
									Č
ATOM	4335		TYR B		21.988	76.664	77.070	1.00 30.79	С
ATOM	4336	CE1	TYR B	184	22.139	73.900	77.159	1.00 41.68	С
MOTA	4337	CE2	TYR B	184	21.590	75.986	78.211	1.00 29.12	С
	4338					74.601	78.255	1.00 39.41	č
ATOM		CZ	TYR B		21.668				
MOTA	4339	ОН	TYR B		21.292	73.927	79.406	1.00 43.60	0
MOTA	4340	N	LYS B	185	24.459	77.784	72.394	1.00 62.31	N
MOTA	4341	CA	LYS B		24.720	77.954	70.961	1.00 71.54	C
						77.639			č
ATOM	4342	C	LYS B		26.173		70.625	1.00 71.35	
MOTA	4343	0	LYS B		26.464	76.800	69.761	1.00 73.96	0
MOTA	4344	СВ	LYS B		24.405	79.395	70.499	1.00 79.89	С
ATOM	4345	CG	LYS B		22.923	79.793	70.468	1.00 90.86	č
									ž
MOTA	4346	CD	LYS B		22.660	81.032	69.585	1.00 94.03	Ċ
MOTA	4347	CE	LYS B	185	23.359	82.293	70.095	1.00 97.96	C
MOTA	4348	NZ	LYS B		23.053	83.504	69.271	1.00 98.03	N
ATOM	4349	N	HIS B		27.077	78.322	71.321	1.00 67.93	N
MOTA	4350	CA	HIS B		28.505	78.151	71.110	1.00 71.49	C
ATOM	4351	С	HIS B	186	28.894	76.678	71.129	1.00 71.96	С
MOTA	4352	ŏ	HIS B		29.289	76.111	70.104	1.00 72.49	0
					29.279	78.910	72.182	1.00 72.20	č
MOTA	4353	CB	HIS B						<u>-</u>
MOTA	4354	CG	HIS B		30.745	79.010	71.908	1.00 80.37	C
ATOM	4355	ND1		186	31.620	79.620	72.777	1.00 80.25	N
ATOM	4356		HIS B		31.489	78.578	70.861	1.00 86.20	С
							72.280		č
ATOM	4357			186	32.844	79.561		1.00 88.39	
MOTA	4358	NE2	HIS B		32.791	78.935	71.119	1.00 92.59	N
MOTA	4359	N	MET B		28.775	76.067	72.302	1.00 67.47	N
ATOM	4360	CA	MET B		29.100	74.656	72.475	1.00 63.47	Ċ
									•

		_		_	107	20 554	77 071	71 701	1 00 56 03	^
MOTA	4361	C	MET	-		28.554	73.831	71.301	1.00 56.92	c
MOTA	4362	0	MET			29.277	73.045	70.680	1.00 54.64	0
ATOM	4363	CB	MET			28.515	74.164	73.811	1.00 60.48	Ç
MOTA	4364	CG	MET	В	187	28.709	72.679	74.112	1.00 69.23	С
MOTA	4365	SD	MET	В	187	30.432	72.124	74.165	1.00 77.92	S
ATOM	4366	CE	MET	В	187	30.791	72.276	75.893	1.00 66.33	С
ATOM	4367	N	SER			27.277	74.043	70.996	1.00 50.98	N
ATOM	4368	CA	SER			26.597	73.348	69.908	1.00 46.97	Ċ
						27.472	73.286	68.668	1.00 45.49	č
ATOM	4369	C	SER							
MOTA	4370	0	SER			27.652	72.227	68.074	1.00 36.98	0
MOTA	4371	CB	SER			25.285	74.059	69.570	1.00 48.08	Ç
ATOM	4372	OG	SER	В	188	24.556	73.339	68.598	1.00 49.12	0
MOTA	4373	N	LEU	В	189	28.022	74.430	68.290	1.00 46.79	N
MOTA	4374	CA	LEU	В	189	28.887	74.523	67.117	1.00 53.44	С
MOTA	4375	C	LEU	В	189	30.231	73.831	67.360	1.00 50.11	С
ATOM	4376	ō	LEU			30.780	73.173	66.466	1.00 48.93	0
	4377	ČВ	LEU			29.129	75.998	66.778	1.00 62.69	č
ATOM	4378		LEU			27.896	76.898	66.612	1.00 69.48	č
ATOM		CG						66.690		č
MOTA	4379		LEU			28.327	78.363		1.00 69.15	Č
ATOM	4380		LEU			27.186	76.588	65.283	1.00 71.03	C
MOTA	4381	N	ALA			30.755	74.001	68.574	1.00 43.50	N
ATOM	4382	CA	ALA	В	190	32.034	73.412	68.955	1.00 46.88	С
ATOM	4383	С	ALA	В	190	32.027	71.929	68.637	1.00 49.66	С
ATOM	4384	0	ALA	В	190	32.967	71.398	68.049	1.00 48.69	0
MOTA	4385	CB	ALA	В	190	32.285	73.630	70.440	1.00 45.92	С
ATOM	4386	Ņ	LEU			30.941	71.271	69.016	1.00 57.32	N
ATOM	4387	ĊΑ	LEU			30.793	69.844	68.780	1.00 64.62	C
							69.508	67.274	1.00 68.59	č
MOTA	4388	č	LEU			30.777		66.791		ŏ
ATOM	4389	0	LEU			31.671	68.806		1.00 73.98	0
MOTA	4390	СВ	LEU			29.521	69.347	69.493	1.00 63.93	c
MOTA	4391	CG	LEU			29.465	69.631	71.015	1.00 63.18	С
MOTA	4392	CD1	LEU	В	191	28.071	69.343	71.552	1.00 66.63	С
ATOM	4393	CD2	LEU	В	191	30.499	68.789	71.762	1.00 52.69	Ċ
MOTA	4394	N	ASN	В	192	29.781	70.018	66.539	1.00 76.65	N
ATOM	4395	CA	ASN			29.656	69.781	65.086	1.00 86.95	С
ATOM	4396	c	ASN			31.027	69.895	64.449	1.00 88.71	Ċ
	4397	ŏ	ASN			31.365	69.184	63.497	1.00 91.35	ō
ATOM						28.704	70.814	64.439	1.00 88.88	č
ATOM	4398	CB	ASN							č
ATOM	4399	CG	ASN			28.620	70.686	62.906	1.00 83.62	
MOTA	4400		ASN			29.534	71.101	62.191	1.00 70.80	0
ATOM	4401	ND2	ASN			27.509	70.116	62.432	1.00 82.55	N
MOTA	4402	N	ARG	В	193	31.812	70.808	65.003	1.00 86.76	N
MOTA	4403	CA	ARG	В	193	33.161	71.071	64.545	1.00 82.47	С
MOTA	4404	C	ARG			34.081	69.885	64.814	1.00 70.87	C
ATOM	4405	ŏ	ARG			34.838	69.474	63.938	1.00 67.90	0
ATOM	4406	СВ	ARG			33.701	72.307	65.253	1.00 88.33	С
						35.004	72.839	64.697	1.00 98.87	č
ATOM	4407	CG	ARG					65.433	1.00112.98	č
MOTA	4408	CD	ARG			35.354	74.104			
ATOM	4409	NE	ARG			34.145	74.896	65.659	1.00124.52	N
MOTA	4410	CZ	ARG			34.084	75.991	66.414	1.00127.47	C
MOTA	4411	NH1	ARG	В	193	35.170	76.445	67.029	1.00125.63	N
ATOM	4412	NH2	ARG	В	193	32.929	76.630	66.562	1.00128.36	N
MOTA	4413	N	THR	В	194	34.010	69.331	66.018	1.00 60.49	N
MOTA	4414	CA	THR	В	194	34.860	68.201	66.373	1.00 56.47	С
ATOM '	4415	Ċ	THR			34.764	67.077	65.358	1.00 54.18	С
MOTA	4416	ŏ	THR			35.707	66.300	65.205	1.00 56.94	0
MOTA	4417	СВ	THR			34.489	67.602	67.738	1.00 62.64	č
							66.885	67.616	1.00 64.36	ŏ
MOTA	4418		THR			33.255		68.788		č
MOTA	4419		THR	_		34.347	68.698		1.00 67.77	N
ATOM	4420	N	GLY			33.626	66.973	64.679	1.00 54.96	
MOTA	4421	CA	GLY			33.473	65.924	63.690	1.00 68.23	c
MOTA	4422	С	GLY	В	195	32.794	64.682	64.229	1.00 74.58	С
ATOM	4423	0	GLY			32.168	63.933	63.478	1.00 79.21	0
MOTA	4424	N	ARG			32.930	64.456	65.531	1.00 75.66	N
ATOM	4425	CA	ARG			32.313	63.305	66.187	1.00 77.42	С
MOTA	4426	C	ARG			30.795	63.529	66.182	1.00 72.79	С
ATOM	4427	ŏ	ARG			30.333	64.637	66.449	1.00 67.36	ō
ATOM	4428	СВ	ARG			32.843	63.194	67.631	1.00 81.41	č
							62.005	68.456	1.00 87.93	č
ATOM	4429	CG	ARG			32.333	60.752	68.294	1.00 90.34	č
ATOM	4430	CD	ARG			33.183				
MOTA	4431	NE	ARG			32.592	59.628	69.015	1.00 94.58	N
MOTA	4432	CZ	ARG			32.916	58.353	68.824	1.00 98.29	C
MOTA	4433	NH1	ARG	В	196	33.839	58.017	67.929	1.00 97.63	N
MOTA	4434	NH2	ARG	В	196	32.296	57.408	69.518	1.00103.72	N
MOTA	4435	N	SER	В	197	30.026	62.494	65.851	1.00 71.16	N
MOTA	4436	CA	SER			28.568	62.600	65.839	1.00 69.64	С
ATOM	4437	C	SER			28.089	62.511	67.289	1.00 69.02	С
ATOM	4438	ŏ	SER			28.034	61.414	67.856	1.00 71.10	0
ATOM	4439	СВ			197	27.959	61.456	65.028	1.00 69.96	Ċ
ATOM	4440	OG			197	28.501	61.421	63.725	1.00 71.61	ō
ATOM	4441	N			198	27.743	63.658	67.882	1.00 65.88	Ň
017	4441	*4	+ 11 [£ 2 0	21.143				**

MOTA	4442	CA	ILE	B 198	27.299	63.712	69.279	1.00 61.80	С
ATOM	4443	C	ILE	B 198	25.866	64.200	69.501	1.00 60.52	С
ATOM	4444	õ		B 198	25.568	65.364	69.259	1.00 60.48	0
ATOM	4445	СВ		B 198	28.200	64.660	70.122	1.00 60.81	С
ATOM	4446			B 198	29.678	64.420	69.815	1.00 65.48	C
ATOM	4447			B 198	27.946	64.427	71.614	1.00 56.41	Ċ
ATOM	4448			B 198	30.607	65.443	70.448	1.00 65.33	č
ATOM	4449	N		B 199	24.979	63.330	69.973	1.00 57.43	N
ATOM	4450	CA		B 199	23.618	63.769	70.260	1.00 49.81	Ċ
ATOM	4451	c		B 199	23.719	64.820	71.351	1.00 43.22	č
MOTA	4452	ŏ		B 199	24.204	64.553	72.451	1.00 41.32	ŏ
MOTA	4453	СВ		B 199	22.740	62.631	70.772	1.00 52.26	č
ATOM	4454			B 199	21.425	63.197	71.298	1.00 52.72	č
ATOM	4455			B 199	22.493	61.636	69.648	1.00 55.82	č
ATOM	4456	N N		B 200	23.257	66.018	71.036	1.00 35.72	Ň
ATOM	4457	CA		B 200	23.331	67.129	71.966	1.00 39.70	Ċ
ATOM	4458	c		B 200	21.998	67.382	72.639	1.00 42.09	č
MOTA	4459	ŏ		B 200	21.038	67.775	71.971	1.00 44.05	ŏ
ATOM	4460	СВ		B 200	23.788	68.359	71.193	1.00 45.19	Č
ATOM	4461	CG		B 200	24.006	69.610	72.004	1.00 47.73	č
ATOM	4462			B 200	24.658	69.570	73.231	1.00 54.60	Č
ATOM	4463			B 200	23.624	70.853	71.500	1.00 46.16	č
ATOM	4464			B 200	24.929	70.743	73.939	1.00 60.84	Ċ
ATOM	4465			B 200	23.888	72.031	72.190	1.00 51.40	Č
ATOM	4466	cz		B 200	24.543	71.974	73.413	1.00 59.57	Ċ
MOTA	4467	ОН		B 200	24.808	73.144	74.102	1.00 58.13	ō
ATOM	4468	N		B 201	21.944	67.147	73.954	1.00 41.10	N
ATOM	4469	CA		B 201	20.719	67.338	74.738	1.00 43.57	ċ
MOTA	4470	c		B 201	20.781	68.543	75.670	1.00 41.63	č
MOTA	4471	ŏ		B 201	21.400	68.500	76.736	1.00 35.40	Ō
ATOM	4472	СB		B 201	20.407	66.103	75.571	1.00 46.88	Ċ
ATOM	4473	OG		B 201	19.239	66.329	76.338	1.00 49.04	Ō
ATOM	4474	N		B 202	20.089	69.600	75.267	1.00 43.09	N
MOTA	4475	CA		B 202	20.062	70.849	76.002	1.00 40.52	С
ATOM	4476	Č.		B 202	19.030	70.884	77.115	1.00 40.12	С
ATOM	4477	ō		B 202	18.131	70.045	77.175	1.00 45.63	0
ATOM	4478	СB		B 202	19.818	71.990	75.018	1.00 39.64	С
ATOM	4479	SG		B 202	20.914	71.849	73.565	1.00 56.69	S
ATOM	4480	N		B 203	19.194	71.865	78.001	1.00 32.53	N
MOTA	4481	CA		B 203	18.317	72.100	79.153	1.00 30.57	С
ATOM	4482	c		B 203	18.027	73.604	79.110	1.00 32.05	С
ATOM	4483	ŏ		B 203	17.406	74.181	80.005	1.00 34.36	0
ATOM	4484	CB		B 203	19.068		80.431	1.00 30.69	С
ATOM	4485	CG		B 203	18.200		81.658	1.00 40.33	С
ATOM	4486	CD		B 203	18.939		82.789	1.00 44.25	С
MOTA	4487			B 203	19.292		82.637	1.00 42.33	0
ATOM	4488			B 203	19.182		83.827	1.00 46.40	0
ATOM	4489	N		B 204	18.498		78.021	1.00 34.86	N
ATOM	4490	CA		B 204	18.369		77.732	1.00 33.77	С
ATOM	4491	C		B 204	17.020		78.159	1.00 33.34	С
ATOM	4492	ō		B 204	16.976		79.038	1.00 32.51	0
ATOM	4493	CB	TRP	B 204	18.597	75.810	76.229	1.00 36.11	С
ATOM	4494	CG	TRP	B 204	18.627	77.212	75.706	1.00 43.38	C
ATOM	4495		TRP	B 204	18.269	78.354	76.361	1.00 52.77	С
ATOM	4496			B 204	19.020	77.613	74.379	1.00 46.69	С
MOTA	4497	NE1	TRP	B 204	18.414	79.439	75.526	1.00 58.54	N
MOTA	4498	CE2	TRP	B 204	18.874	79.012	74.305	1.00 53.83	С
MOTA	4499			B 204	19.483		73.248	1.00 44.22	Ç
MOTA	4500	CZ2	TRP	B 204	19.177	79.737	73.144	1.00 57.36	С
MOTA	4501	CZ3	TRP	B 204	19.785		72.096	1.00 42.79	Ç
MOTA	4502	CH2	TRP	B 204	19.630		72.055	1.00 51.56	С
MOTA	4503	N	PRO	B 205	15.902		77.562	1.00 35.29	N
ATOM	4504	CA	PRO	B 205	14.556		77.851	1.00 24.59	Č
MOTA	4505	С		B 205	14.260		79.332	1.00 20.83	Ç
ATOM	4506	0		B 205	13.889		79.825	1.00 28.83	0
MOTA	4507	CB		B 205	13.644		77.163	1.00 28.26	Ç
ATOM	4508	CG		B 205	14.485		76.070	1.00 39.15	C
ATOM	4509	CD		B 205	15.813		76.754	1.00 41.80	C
ATOM	4510	N		B 206	14.382		80.025	1.00 15.54	N
ATOM	4511	CA		B 206	14.127		81.457	1.00 24.00	C
MOTA	4512	ç		B 206	14.743		82.164	1.00 26.77	C
ATOM	4513	0		B 206	14.303		83.250	1.00 19.16	C 0
ATOM	4514	CB		B 206	14.724		82.018	1.00 35.69	c
ATOM	4515	CG		B 206	14.832		83.539	1.00 49.18	Ċ
MOTA	4516			B 206	13.444		84.157	1.00 60.58	c
ATOM	4517			B 206	15.662		83.925	1.00 59.26	N
ATOM	4518	N		B 207	15.770		81.531 82.046	1.00 38.18	C
MOTA	4519	CA		B 207	16.477		81.372	1.00 48.47 1.00 58.12	č
ATOM	4520	C		B 207	16.156		81.756	1.00 58.12	Ö
ATOM	4521	0		B 207	16.712		81.985	1.00 50.26	č
MOTA	4522	СВ	111	B 207	17.981		01.703	1.00 30.20	·

MOTA	4523	CG	TYR	B 207	18.439	76.924	83.008	1.00 54.09	С
ATOM	4524			B 207	18.521		84.349	1.00 53.33	С
ATOM	4525			B 207	18.748		82.645	1.00 57.56	Ċ
									č
ATOM	4526			B 207	18.900		85.313	1.00 55.47	
ATOM	4527	CE2	TYR	B 207	19.129	74.675	83.598	1.00 56.42	. с
MOTA	4528	CZ	TYR	B 207	19.201	75.039	84.931	1.00 54.59	С
ATOM	4529	ОН	TYR	B 207	19.553	74.099	85.877	1.00 54.11	0
ATOM	4530	N	MET		15.289		80.362	1.00 67.16	N
									Ĉ
ATOM	4531	CA		B 208	14.937		79.736	1.00 76.35	
MOTA	4532	С	MET	B 208	13.915	81.470	80.644	1.00 81.72	С
ATOM	4533	0	MET	B 208	13.966	82.692	80.809	1.00 85.11	0
ATOM	4534	CB		B 208	14.380		78.327	1.00 78.86	С
ATOM	4535	CG		B 208	15.418		77.277	1.00 78.81	Č
								1.00 93.07	Š
ATOM	4536	SD		B 208	14.772		75.613		
ATOM	4537	CE		B 208	14.251		75.607	1.00 86.49	C
MOTA	4538	N	TRP	B 209	13.008	80.687	81.235	1.00 86.64	N
ATOM	4539	CA	TRP	B 209	12.029	81.188	82.189	1.00 96.02	С
MOTA	4540	С	TRP	B 209	12.995		83.364	1.00101.19	С
ATOM	4541	ō		B 209	13.911		83.551	1.00 99.10	0
								1.00102.01	č
ATOM	4542	СВ		B 209	11.041		82.612		
ATOM	4543	CG		B 209	10.043		81.557	1.00107.53	C
MOTA	4544	CD1	TRP	B 209	9.016	80.384	81.049	1.00109.21	С
MOTA	4545	CD2	TRP	B 209	10.005	78.368	80.855	1.00107.49	С
ATOM	4546			B 209	8.345		80.072	1.00107.06	N
	4547			B 209	8.938		79.929	1.00105.86	Ċ
MOTA								1.00104.86	č
MOTA	4548			B 209	10.773		80.918		
MOTA	4549	CZ2	TRP	B 209	8.625	77.374	79.067	1.00100.39	С
MOTA	4550	CZ3	TRP	B 209	10.456	76.143	80.063	1.00101.89	С
MOTA	4551	CH2	TRP	B 209	9.390	76.245	79.147	1.00 99.66	С
MOTA	4552	N		B 210	12.826		84.153	1.00106.91	N
				B 210	11.842		84.165	1.00114.58	Ċ
MOTA	4553	CA							č
MOTA	4554	С	PRO		12.358		83.452	1.00119.07	
MOTA	4555	0	PRO	B 210	12.703		84.096	1.00120.59	0
ATOM	4556	CB	PRO	B 210	11.676	83.859	85.634	1.00112.27	С
MOTA	4557	CG	PRO	B 210	13.093	83.768	86.118	1.00111.13	С
ATOM	4558	CD	PRO		13.587		85.420	1.00107.22	С
	4559			B 211	12.402		82.132	1.00123.20	N
MOTA		N							
MOTA	4560	CA		B 211	12.904		81.361	1.00125.20	C
ATOM	4561	С	PHE	B 211	12.062		80.138	1.00121.76	С
MOTA	4562	0	PHE	B 211	11.730	87.225	79.797	1.00125.34	0
MOTA	4563	CB		B 211	14.348	85.590	80.957	1.00132.80	С
ATOM	4564	ĊĞ		B 211	15.322		82.093	1.00141.06	С
								1.00143.96	č
MOTA	4565			B 211	15.621		82.673		
ATOM	4566		PHE		15.957		82.570	1.00143.20	c
ATOM	4567	CEl	PHE	B 211	16.539	86.999	83.709	1.00147.62	С
ATOM	4568	CE2	PHE	B 211	16.872	84.622	83.605	1.00144.40	С
ATOM	4569	CZ	PHE		17.169		84.175	1.00147.42	С
ATOM	4570	N	GLN		11.714		79.475	1.00117.65	N
							78.262	1.00116.10	Ċ
ATOM	4571	CA		B 212	10.899				Č
ATOM	4572	С	GLN		10.741		77.630	1.00113.23	
ATOM	4573	0	GLN		11.690		77.603	1.00113.03	0
ATOM	4574	CB	GLN	B 212	11.539	86.026	77.266	1.00122.76	С
MOTA	4575	CG	GLN	B 212	13.060	86.006	77.235	1.00126.97	С
ATOM	4576	CD	GLN		13.638		76.347	1.00128.58	С
ATOM	4577		GLN		13.426		76.596	1.00128.76	0
							75.293	1.00129.44	N
MOTA	4578			B 212	14.351				N N
MOTA	4579	N	LYS		9.541		77.135	1.00111.73	
ATOM	4580	CA	LYS	B 213	9.236	82.153	76.480	1.00112.52	C
ATOM	4581	С	LYS	B 213	10.25	81.991	75.330	1.00107.11	С
ATOM	4582	0		B 213	10.427	82.887	74.515	1.00108.90	0
ATOM	4583	ĊВ		B 213	7.788		75.936	1.00116.60	С
				B 213	6.72		76.979	1.00118.58	C
ATOM	4584	CG					77.061	1.00115.90	č
ATOM	4585	CD		B 213	6.52				
ATOM	4586	CE		B 213	5.279		77.879	1.00111.08	C
MOTA	4587	NZ	LYS	B 213	5.070	85.985	78.035	1.00 99.14	N
MOTA	4588	N	PRO	B 214	10.960	80.848	75.278	1.00 99.46	N
ATOM	4589	CA		B 214	11.98		74.269	1.00 94.71	С
ATOM	4590	c		B 214	11.71		72.754	1.00 90.00	Č
							72.317	1.00 92.92	ŏ
ATOM	4591	0		B 214	10.69				č
MOTA	4592	CB		B 214	12.547		74.803	1.00 96.49	Č
MOTA	4593	CG		B 214	11.51		75.811	1.00 90.86	C
ATOM	4594	CD	PRO	B 214	10.99	79.920	76.431	1.00 92.17	С
ATOM	4595	N		B 215	12.63		71.961	1.00 82.14	N
ATOM	4596	CA		B 215	12.49		70.510	1.00 73.32	· c
					12.89	-	70.336	1.00 62.81	č
ATOM	4597	Ç		B 215			70.282	1.00 53.18	õ
ATOM	4598	0		B 215	14.07				ŏ
MOTA	4599	CB		B 215	13.50		69.779	1.00 86.68	c
MOTA	4600	CG		B 215	13.27		68.254	1.00 96.59	c
MOTA	4601	OD1		B 215	12.63		67.692	1.00 97.37	0
MOTA	4602			B 215	13.79		67.596	1.00105.86	N
ATOM	4603	N		B 216	11.89		70.342	1.00 56.91	N
	_								

ATOM	4604	CA	TVR	B 216	12.095	77.143	70.169	1.00 57.71	С
ATOM	4605	c		B 216	12.577	76.824	68.756	1.00 58.93	č
				_ : : :					
MOTA	4606	0		B 216	13.278	75.834	68.532	1.00 66.37	0
MOTA	4607	CB		B 216	10.786	76.387	70.436	1.00 54.68	С
MOTA	4608	CG	TYR	B 216	10.478	76.145	71.908	1.00 47.31	С
MOTA	4609	CD1	TYR	B 216	11.306	75.331	72.695	1.00 48.30	С
MOTA	4610			B 216	9.350	76.709	72.511	1.00 45.03	Ċ
ATOM	4611			B 216	11.017	75.082	74.040	1.00 38.66	č
MOTA	4612			B 216	9.054	76.466	73.860	1.00 39.11	Ç
MOTA	4613	CZ	TYR	B 216	9.893	75.650	74.615	1.00 36.71	С
ATOM	4614	ОН	TYR	B 216	9.606	75.397	75.945	1.00 39.39	0
ATOM	4615	N	THR	B 217	12.194	77.650	67.791	1.00 58.65	N
ATOM	4616	CA		B 217	12.629	77.407	66.425	1.00 64.38	С
ATOM	4617	c		B 217	14.141	77.577	66.435	1.00 63.38	č
MOTA	4618	0_		B 217	14.868	76.880	65.723	1.00 70.77	0
MOTA	4619	СВ		B 217	11.998	78.419	65.456	1.00 72.29	Ç
MOTA	4620	OG1	THR	B 217	10.586	78.492	65.704	1.00 71.64	0
MOTA	4621	CG2	THR	B 217	12.225	77.985	64.015	1.00 78.78	С
ATOM	4622	N	GLU	B 218	14.595	78.516	67.259	1.00 60.24	N
MOTA	4623	CA		B 218	16.009	78.808	67.407	1.00 59.38	Ċ
									č
ATOM	4624	C		B 218	16.657	77.568	67.994	1.00 53.71	_
MOTA	4625	0		B 218	17.401	76.857	67.320	1.00 46.21	0
MOTA	4626	CB		B 218	16.163	79.999	68.345	1.00 62.05	С
ATOM	4627	CG	GLU	B 218	17.578	80.397	68.675	1.00 71.15	С
ATOM	4628	CD		B 218	17.702	81.896	68.856	1.00 77.94	С
MOTA	4629			B 218	17.520	82.623	67.851	1.00 79.20	ō
	4630			B 218	17.967	82.349	69.993	1.00 76.55	ŏ
ATOM									
ATOM	4631	N		B 219	16.342	77.320	69.259	1.00 49.61	N
MOTA	4632	CA		B 219	16.840	76.171	70.011	1.00 41.53	С
MOTA	4633	С	ILE	B 219	16.924	74.897	69.185	1.00 34.04	С
ATOM	4634	0	ILE	B 219	17.939	74.208	69.199	1.00 38.58	0
MOTA	4635	CB		B 219	15.922	75.870	71.204	1.00 40.80	С
ATOM	4636			B 219	15.813	77.115	72.089	1.00 48.95	Ċ
					16.433	74.653	71.967	1.00 35.42	č
ATOM	4637			B 219					
MOTA	4638			B 219	15.161	76.865	73.432	1.00 53.55	C
MOTA	4639	N		B 220	15.832	74.582	68.492	1.00 25.48	N
ATOM	4640	CA	ARG	B 220	15.742	73.393	67.662	1.00 31.02	С
MOTA	4641	С	ARG	B 220	16.849	73.364	66.627	1.00 38.66	С
MOTA	4642	ŏ		B 220	17.166	72.310	66.083	1.00 43.62	0
				B 220	14.380	73.329	66.964	1.00 38.15	č
ATOM	4643	CB							č
MOTA	4644	CG		B 220	14.388	72.450	65.737	1.00 54.45	C
ATOM	4645	CD	ARG	B 220	13.016	71.956	65.382	1.00 70.29	С
ATOM	4646	NE	ARG	B 220	13.095	70.576	64.916	1.00 91.96	N
MOTA	4647	CZ	ARG	B 220	12.040	69.823	64.626	1.00 98.73	С
ATOM	4648			B 220	10.817	70.322	64.753	1.00100.04	N
ATOM	4649			B 220	12.206	68.570	64.218	1.00102.81	N
								1.00 47.73	N
ATOM	4650	N		B 221	17.428	74.524	66.340		
MOTA	4651	CA		B 221	18.513	74.597	65.368	1.00 59.37	C
MOTA	4652	С	GLN	B 221	19.827	74.423	66.097	1.00 58.36	С
ATOM	4653	0	GLN	B 221	20.897	74.725	65.565	1.00 63.76	0
MOTA	4654	CB	GLN	B 221	18.542	75.951	64.681	1.00 68.87	С
ATOM	4655	CG	GLN	B 221	17.296	76.321	63.945	1.00 83.58	С
ATOM	4656	CD	GLN		17.505	77.570	63.134	1.00 91.32	С
ATOM	4657			B 221	17.891	78.617	63.665	1.00 94.94	ŏ
								1.00 91.81	N
ATOM	4658		GLN		17.261	77.471	61.836		
ATOM	4659	N	TYR		19.741	73.938	67.325	1.00 52.75	N
MOTA	4660	CA	TYR		20.930	73.751	68.141	1.00 49.86	Č
ATOM	4661	С	TYR	B 222	20.885	72.521	69.047	1.00 51.82	С
ATOM	4662	0	TYR	B 222	21.879	72.193	69.693	1.00 56.44	0
ATOM	4663	CB		B 222	21.149	74.991	69.008	1.00 52.48	С
ATOM	4664	CG		B 222	21.678	76.187	68.266	1.00 62.64	С
ATOM	4665			B 222	22.894	76.126	67.596	1.00 67.88	č
	4666			B 222	20.988	77.393	68.275	1.00 63.36	č
MOTA									č
ATOM	4667			B 222	23.415	77.230	66.960	1.00 68.70	0000
MOTA	4668	CE2		B 222	21.499	78.509	67.642	1.00 66.58	Ē
MOTA	4669	CZ		B 222	22.717	78.418	66.988	1.00 65.02	С
MOTA	4670	ОН	TYR	B 222	23.259	79.516	66.372	1.00 63.49	0
MOTA	4671	N		B 223	19.746	71.837	69.100	1.00 50.96	N
MOTA	4672	CA		B 223	19.640	70.683	69.973	1.00 48.83	С
MOTA	4673	c		B 223	18.857	69.531	69.418	1.00 49.05	C
MOTA	4674	ŏ		B 223	17.946	69.709	68.616	1.00 52.90	ŏ
								1.00 51.12	č
MOTA	4675	CB		B 223	19.011	71.113	71.279		
MOTA	4676	SG		B 223	19.851	72.564	71.979	1.00 53.29	S
MOTA	4677	N		B 224	19.214	68.338	69.866	1.00 45.96	N
MOTA	4678	CA	ASN	B 224	18.523	67.137	69.433	1.00 44.72	С
ATOM	4679	С		B 224	17.286	66.968	70.324	1.00 37.77	С
ATOM	4680	ō		B 224	16.319	66.280	69.974	1.00 39.98	0
ATOM	4681	СB		B 224	19.478	65.956	69.528	1.00 51.18	č
ATOM	4682	CG		B 224	20.587	66.052	68.520	1.00 58.33	č
ATOM	4683			B 224	21.754	65.840	68.836	1.00 65.65	ō
						66.373	67.286	1.00 56.79	N N
ATOM	4684	NUZ	MON	B 224	20.226	00.313	07.200	1.00 30.79	IV

				_	225		CO COO			
MOTA	4685	N	HIS			17.343	67.609	71.485	1.00 31.45	N
MOTA	4686	CA	HIS	В	225	16.245	67.631	72.427	1.00 33.69	С
MOTA	4687	С	HIS	R	225	16.642	68.400	73.660	1.00 32.39	С
			HIS			17.776				ŏ
MOTA	4688	0					68.344	74.121	1.00 30.58	
MOTA	4689	CB	HIS			15.721	66.235	72.763	1.00 36.06	С
MOTA	4690	CG	HIS	В	225	16.774	65.182	72.887	1.00 34.13	С
MOTA	4691	NDI	HIS	В	225	17.674	65.148	73.929	1.00 29.91	N
					225	17.014		72.141	1.00 33.57	Ċ
MOTA	4692	CD2					64.075			
ATOM	4693		HIS			18.419	64.061	73.823	1.00 27.98	С
MOTA	4694	NE2	HIS	В	225	18.039	63.393	72.749	1.00 27.97	N
ATOM	4695	N	TRP			15.667	69.126	74.179	1.00 32.53	N
		CA	TRP			15.839	70.025	75.307	1.00 33.97	Ċ
ATOM	4696									
ATOM	4697	С	TRP			14.852	69.787	76.464	1.00 38.96	Ç
ATOM	4698	0	TRP	В	226	13.775	69.221	76.275	1.00 47.80	0
ATOM	4699	CB	TRP	В	226	15.653	71.435	74.754	1.00 30.08	С
ATOM	4700	ĊĠ	TRP			14.415	71.478	73.872	1.00 32.05	C
									1.00 32.11	č
ATOM	4701		TRP			13.112	71.579	74.293		
MOTA	4702	CD2	TRP	В	226	14.354	71.268	72.451	1.00 31.67	С
MOTA	4703	NE1	TRP	В	226	12.251	71.438	73.226	1.00 23.57	N
ATOM	4704	CE2	TRP	В	226	12.983	71.244	72.087	1.00 28.32	С
	4705		TRP			15.322	71.090	71.450	1.00 39.08	Ċ
ATOM										. č
MOTA	4706		TRP			12.557	71.053	70.768	1.00 33.66	
MOTA	4707	CZ3	TRP	В	226	14.894	70.896	70.125	1.00 50.47	С
MOTA	4708	CH2	TRP	В	226	13.521	70.879	69.803	1.00 47.28	C
MOTA	4709	N	ARG	В	227	15.229	70.239	77.658	1.00 31.64	N
	4710	CA	ARG			14.389	70.117	78.849	1.00 35.03	C
ATOM								_		
MOTA	4711	С	ARG			13.435	71.312	78.913	1.00 39.53	Č
ATOM	4712	0	ARG	В	227	13.776	72.405	78.461	1.00 40.49	0
ATOM	4713	CB	ARG	В	227	15.259	70.096	80.106	1.00 35.87	С
ATOM	4714	CG	ARG			15.897	68.764	80.394	1.00 35.40	С
									1.00 38.85	č
ATOM	4715	CD	ARG			14.850	67.753	80.848		
MOTA	4716	NE	ARG			14.285	68.071	82.155	1.00 27.21	Ŋ
ATOM	4717	CZ	ARG	В	227	14.982	68.090	83.284	1.00 24.17	С
ATOM	4718	NH1	ARG	В	227	16.274	67.809	83.276	1.00 23.16	N
ATOM	4719	NH2	ARG			14.384	68.385	84.423	1.00 21.24	N
										N
MOTA	4720	N	ASN			12.243	71.107	79.470	1.00 39.75	
MOTA	4721	CA	ASN	В	228	11.268	72.189	79.579	1.00 37.24	С
MOTA	4722	С	ASN	В	228	10.850	72.435	81.025	1.00 43.45	С
ATOM	4723	0	ASN			10.843	73.587	81.472	1.00 51.94	0
						10.008	71.900	78.745	1.00 40.38	Ċ
ATOM	4724	СВ	ASN							
MOTA	4725	CG	ASN			10.285	71.836	77.249	1.00 53.86	Č
MOTA	4726	OD1	ASN	В	228	10.999	72.675	76.697	1.00 55.95	0
MOTA	4727	ND2	ASN	В	228	9.704	70.839	76.582	1.00 65.88	N
	4728		PHE			10.509	71.359	81.751	1.00 49.79	N
ATOM		N								
MOTA	4729	CA	PHE			10.057	71.446	83.155	1.00 47.88	C
ATOM	4730	С	PHE	В	229	11.022	70.869	84.201	1.00 44.13	С
MOTA	4731	0	PHE	В	229	11.804	69.960	83.911	1.00 45.53	0
ATOM	4732	CB	PHE			8.696	70.755	83.318	1.00 51.04	С
								84.648	1.00 68.22	č
ATOM	4733	CG	PHE			8.043	71.005			č
ATOM	4734		PHE			7.596	72.281	84.986	1.00 77.87	c
ATOM	4735	CD2	PHE	В	229	7.889	69.974	85.572	1.00 79.81	С
ATOM	4736	CE1	PHE	В	229	7.005	72.528	86.224	1.00 86.97	С
ATOM	4737	CE2				7.296	70.210	86.819	1.00 86.80	С
							·71.486	87.143	1.00 90.80	č
MOTA	4738	CZ			229	6.856				
ATOM	4739	N	ALA	В	230	10.930	71.403	85.422	1.00 42.28	N
ATOM	4740	CA	ALA	В	230	11.769	71.006	86.564	1.00 47.28	С
ATOM	4741	C	ALA			12.075	69.521	86.634	1.00 50.55	C
ATOM	4742	ŏ	ALA			11.433	68.708	85.963	1.00 57.81	0
						11.120	71.448	87.869	1.00 46.60	Č
ATOM	4743	СВ	ALA	•	230					N
ATOM	4/44	N	ASP			13.053	69.164	87.461	1.00 46.30	
MOTA	4745	CA	ASP	В	231	13.424	67.762	87.602	1.00 47.24	С
ATOM	4746	С	ASP	В	231	12.220	66.911	87.964	1.00 44.91	С
ATOM	4747	ŏ	ASP			11.121	67.419	88.208	1.00 46.32	0
									1.00 56.16	č
ATOM	4748	CB	ASP			14.501	67.605	88.664		<u> </u>
ATOM	4749	CG	ASP			15.725	68.403	88.334	1.00 61.99	c
ATOM	4750	OD1	ASP	В	231	16.186	68.271	87.185	1.00 64.34	0
ATOM	4751		ASP			16.221	69.159	89.195	1.00 73.15	0
	4752				232	12.436	65.606	88.006	1.00 36.13	Ň
ATOM		N								Ċ
ATOM	4753	CA	ILE			11.354	64.693	88.314	1.00 27.43	Č
ATOM	4754	С			232	11.698	63.756	89.482	1.00 27.62	Ċ
ATOM	4755	0			232	12.726	63.073	89.471	1.00 26.64	0
ATOM	4756	ČВ			232	10.969	63.897	87.022	1.00 25.17	Ċ
						9.834	62.915	87.311	1.00 17.61	ř
MOTA	4757		ILE							C C C
MOTA	4758		ILE			12.195	63.188	86.475	1.00 37.00	Ē.
ATOM	4759	CD1	ILE			9.209	62.355	86.047	1.00 34.79	
MOTA	4760	N	ASP	В	233	10.830	63.768	90.495	1.00 33.04	N
ATOM	4761	CA			233	10.977	62.935	91.687	1.00 34.79	С
MOTA	4762					10.447	61.553	91.370	1.00 30.20	č
		c			233					
MOTA	4763	0			233	9.785	61.362	90.351	1.00 28.34	0
MOTA	4764	CB			233	10.136	63.467	92.850	1.00 50.15	C
MOTA	4765	CG	ASP	В	233	10.531	64.860	93.286	1.00 67.23	С

MOTA	4766	OD1	ASP	В	233	11.660	65.043	93.798	1.00 73.80	0
MOTA	4767		ASP		233	9.697	65.777	93.116	1.00 75.06	0
MOTA	4768	N	ASP		234	10.733	60.587	92.238	1.00 28.34	N
MOTA	4769	CA	ASP		234	10.209	59.244	92.032	1.00 26.19	C
ATOM ATOM	4770 4771	C 0	ASP ASP		234	8.867 8.659	59.339 58.735	92.747 93.803	1.00 24.68	0 C
MOTA	4772	СВ	ASP			11.113	58.198	92.688	1.00 25.05	č
ATOM .	4773	CG	ASP		234	10.676	56.787	92.372	1.00 27.09	Ċ
MOTA	4774		ASP		234	9.949	56.597	91.363	1.00 31.30	0
ATOM	4775		ASP		234	11.062	55.871	93.127	1.00 21.84	0
MOTA MOTA	4776 4777	N CA	SER SER			7.970 6.661	60.131 60.390	92.160 92.743	1.00 25.37	N C
ATOM	4778	c	SER			5.562	60.595	91.718	1.00 28.46	č
MOTA	4779	ō	SER			5.818	61.008	90.589	1.00 32.06	0
MOTA	4780	CB	SER			6.752	61.654	93.595	1.00 29.39	Ç
MOTA	4781	OG	SER			7.218	62.732	92.785	1.00 23.53	0
ATOM	4782	N	TRP TRP			4.329 3.177	60.339 60.532	92.137 91.265	1.00 22.81	N C
ATOM ATOM	4783 4784	CA C	TRP			2.977	62.036	91.038	1.00 28.40	č
ATOM	4785	ŏ	TRP			2.758	62.487	89.909	1.00 31.87	ō
ATOM	4786	CB	TRP			1.933	59.917	91.911	1.00 33.78	С
MOTA	4787	CG	TRP			0.644	60.043	91.126	1.00 33.53	C
MOTA	4788		TRP			-0.602	60.219	91.645	1.00 34.90	C C
MOTA MOTA	4789 4790		TRP		236	0.473 -1.540	59.964 60.256	89.701 90.640	1.00 22.72	N
ATOM	4791		TRP			-0.910	60.101	89.436	1.00 24.75	С
MOTA	4792		TRP		236	1.350	59.791	88.623	1.00 36.82	С
MOTA	4793		TRP		236	-1.441	60.070	88.142	1.00 24.24	Č
ATOM	4794		TRP			0.824	59.760	87.329	1.00 38.70	C
ATOM	4795		TRP LYS			-0.565 3.080	59.900 62.805	87.104 92.116	1.00 28.28 1.00 30.75	C N
ATOM ATOM	4796 4797	N CA	LYS			2.923	64.252	92.053	1.00 35.49	Č
ATOM	4798	Ċ	LYS			3.789	64.840	90.948	1.00 36.92	č
ATOM	4799	ō	LYS			3.280	65.428	89.989	1.00 39.03	0
MOTA	4800	CB	LYS		237	3.320	64.871	93.388	1.00 43.96	Ċ
ATOM	4801	CG	LYS			3.204	66.381	93.443	1.00 58.69	· c
ATOM	4802	CD	LYS LYS			3.590 3.428	66.884 68.388	94.820 94.940	1.00 76.84	C C
ATOM ATOM	4803 4804	CE NZ	LYS			3.684	68.844	96.338	1.00 87.61	N
ATOM	4805	N	SER			5.100	54.667	91.091	1.00 38.16	· N
ATOM	4806	CA	SER			6.061	65.178	90.121	1.00 40.77	С
MOTA	4807	C	SER			5.616	64.875	88.690	1.00 37.84	c
ATOM	4808	0	SER			5.765	65.703	87.781	1.00 44.27	0 C
ATOM ATOM	4809 4810	CB OG	SER SER			7.437 8.409	64.566 65.123	90.376 89.508	1.00 37.16 1.00 54.89	0
ATOM	4811	N	ILE			5.049	63.694	88.483	1.00 27.75	N
MOTA	4812	CA	ILE			4.592	63.343	87.150	1.00 28.70	С
MOTA	4813	С	ILE			3.340	64.110	86.775	1.00 26.04	c
ATOM	4814	0	ILE			3.253	64.682	85.684	1.00 17.63	0
MOTA	4815 4816	CB CG1	ILE			4.349 5.690	61.829 61.148	87.021 86.726	1.00 22.63 1.00 25.11	: C
ATOM ATOM	4817	CG2	ILE			3.303	61.545	85.948	1.00 11.50	č
ATOM	4818	CD1				5.586	59.747	86.171	1.00 25.16	С
MOTA	4819	N	LYS	В	240	2.376	64.134	87.684	1.00 31.73	N
ATOM	4820	CA	LYS			1.145	64.849	87.425	1.00 41.99	c
MOTA MOTA	4821 4822	C 0	LYS			1.461 1.015	66.274 66.704	86.976 85.908	1.00 43.08	C 0
ATOM	4823	СВ	LYS			0.289	64.859	88.683	1.00 47.78	č
ATOM	4824	CG	LYS			-0.052	63.468	89.175	1.00 53.75	č
MOTA	4825	CD	LYS	В	240	-0.659	63.497	90.570	1.00 53.18	С
MOTA	4826	CE	LYS			-1.933	64.328	90.600	1.00 59.78	C
ATOM	4827	NZ	LYS			-2.566 2.252	64.347 66.996	91.950 87.769	1.00 55.99 1.00 43.28	N N
ATOM ATOM	4828 4829	N CA	SER SER			2.252	68.374	87.428	1.00 45.26	C
ATOM	4830	C	SER			3.186	68.483	86.026	1.00 43.14	č
ATOM	4831	Õ	SER			2.803	69.375	85.274	1.00 49.64	0
MOTA	4832	CB	SER	В	241	3.578	68.960	88.445	1.00 48.56	C
ATOM	4833	OG	SER			. 4.779	68.217	88.500	1.00 59.61	0
MOTA MOTA	4834 4835	N CA	ILE			4.099 4.690	67.583 67.616	85.665 84.323	1.00 37.40	N C
ATOM	4836	C			242	3.611	67.464	83.253	1.00 31.73	č
ATOM	4837	ŏ	ILE			3.588	68.217	82.268	1.00 25.40	0
MOTA	4838	СВ	ILE			5.773	66.514	84.142	1.00 32.20	C
MOTA	4839		ILE			7.107	67.024	84.694 82.674	1.00 39.49	c c
MOTA MOTA	4840 4841		ILE			5.928 8.265	66.132 66.077	84.492	1.00 21.06	c
ATOM.	4842	N	LEU			2.714	66.499	83.431	1.00 28.87	Ñ
MOTA	4843	CA	LEU	В	243	1.648	66.344	82.450	1.00 26.17	C
ATOM	4844	C	LEU			0.873	67.651	82.388	1.00 23.84	C
MOTA MOTA	4845	0			243	0.876	68.329 65.202	81.356 82.827	1.00 7.14 1.00 26.24	0 C
A I OF	4846	CB	LEU	٥	243	0.714	05.202	02.021	2.00 20.24	C

HOTA	4847	CG	LEU B 24	3 1.200	63.829	82.375	1.00 21.83	С
MOTA	4848		LEU B 24		62.810	82.822	1.00 22.96	č
MOTA	4849		LEU B 24		63.778	80.866	1.00 28.88	č
	4850	N	ASP B 24			83.500	1.00 20.78	Ñ
MOTA		CA	ASP B 24		68.014	83.558	1.00 28.25	Ċ
MOTA	4851				69.248			c
ATOM	4852	Č	ASP B 24		70.423	82.951	1.00 32.60	
MOTA	4853	0	ASP B 24		71.147	82.105	1.00 37.00	0
MOTA	4854	CB	ASP B 24		69.550	85.001	1.00 31.66	C
HOTA	4855	CC	ASP B 24		68.410	85.626	1.00 33.89	C
MOTA	4856	OD1	ASP B 24	4 -2.683	67.938	84.993	1.00 35.75	0
MOTA	4857	OD2	ASP B 24	4 -1.367	67.978	86.743	1.00 41.32	0
ATOM	4858	N	TRP B 24	5 1.462	70.603	83.372	1.00 38.51	N
MOTA	4859	CA	TRP B 24		71.679	82.845	1.00 46.62	С
MOTA	4860	Ċ	TRP B 24		71.533	81.321	1.00 46.46	c
ATOM	4861	ō	TRP B 24		72.465	80.582	1.00 49.26	ō
MOTA	4862	СB	TRP B 24		71.636	83.443	1.00 61.17	č
ATOM	4863	CG	TRP B 24		72.799	83.004	1.00 88.13	č
ATOM	4864		TRP B 24		74.028	83.594	1.00 96.89	č
			TRP B 24				1.00 99.28	Ċ
MOTA	4865	CD2			72.883	81.813		
MOTA	4866	NE1	TRP B 24		74.877	82.839	1.00106.39	N
MOTA	4867	CE2	TRP B 24		74.198	81.741	1.00105.58	c
MOTA	4868	CE3	TRP B 24		71.976	80.797	1.00102.70	С
MOTA	4869	CZ2	TRP B 24	6.660	74.628	80.691	1.00110.26	С
ATOM	4870	CZ3	TRP B 24	5 6.473	72.403	79.753	1.00103.34	С
ATOM	4871	CH2	TRP B 24	5 6.964	73.718	79.709	1.00110.36	С
ATOM	4872	N	THR B 24	5 2.812	70.371	80.844	1.00 47.19	N
ATOM	4873	CA	THR B 24		70.160	79.404	1.00 48.24	С
ATOM	4874	c	THR B 24		70.300	78.758	1.00 51.43	č
ATOM	4875	ò	THR B 24		70.935	77.707	1.00 53.04	ŏ
MOTA	4876	CB	THR B 24		68.766	79.078	1.00 45.41	č
							1.00 51.10	ō
ATOM	4877	0G1	THR B 24		68.922	78.749		
MOTA	4878	CG2			68.115	77.901	1.00 42.75	C
MOTA	4879	N	SER B 24		69.725	79.406	1.00 52.71	N
MOTA	4880	CA	SER B 24		69.780	78.901	1.00 54.33	Ç
MOTA	4881	С	SER B 24	7 -1.222	71.219	78.577	1.00 52.57	С
ATOM	4882	0	SER B 24	7 -1.774	71.503	77.494	1.00 46.52	0
ATOM	4883	CB	SER B 24	7 -1.796	69.205	79.939	1.00 58.27	C
ATOM	4884	OG	SER B 24	7 -3.072	69.010	79.379	1.00 68.82	0
ATOM	4885	N	PHE B 24		72.113	79.520	1.00 52.38	N
ATOM	4886	CA	PHE B 24		73.541	79.384	1.00 53.08	C
ATOM	4887	C	PHE B 24		74.345	78.707	1.00 47.47	Č
MOTA	4888	ŏ	PHE B 24		75.415	79.167	1.00 48.64	ŏ
		СВ			74.131	80.768	1.00 62.47	č
MOTA	4889		PHE B 24					Č
ATOM	4890	CG	PHE B 24		75.640	80.797	1.00 67.88	Č
MOTA	4891		PHE B 24		76.342	79.962	1.00 77.15	C
MOTA	4892		PHE B 24		76.361	81.617	1.00 60.79	c
ATOM	4893		PHE B 24		77.747	79.943	1.00 78.98	Č
MOTA	4894	CE2	PHE B 24		77.757	81.608	1.00 70.08	C
MOTA	4895	CZ	PHE B 24		78.451	80.769	1.00 78.87	С
ATOM	4896	N	ASN B 24	9 0.487	73.824	77.613	1.00 40.98	N
ATOM	4897	CA	ASN B 24	9 1.528	74.549	76.903	1.00 36.61	C
MOTA	4898	С	ASN B 24	9 1.728	74.118	75.475	1.00 41.21	С
ATOM	4899	0	ASN B 24	9 2.398	74.802	74.715	1.00 37.57	0
ATOM	4900	CB	ASN B 24		74.459	77.642	1.00 32.34	С
ATOM	4901	CG	ASN B 24		75.579	78.621	1.00 39.45	С
MOTA	4902		ASN B 24		76.741	78.280	1.00 53.83	ō
MOTA	4903		ASN B 24		75.245	79.842	1.00 32.18	N
ATOM	4904	N	GLN B 25		72.990	75.106	1.00 51.49	N
		CA			72.473	73.748	1.00 54.53	Ċ
ATOM	4905	_	GLN B 25		73.562	72.680	1.00 56.62	Č
ATOM	4906	Ċ	GLN B 25					
ATOM	4907	0	GLN B 25		73.429	71.745	1.00 58.26	0
MOTA	4908	CB	GLN B 25		71.532	73.428	1.00 52.25	C
ATOM	4909	CG	GLN B 25		71.642	74.400	1.00 46.12	C
ATOM	4910	CD	GLN B 25		70.521	74.223	1.00 42.95	C
MOTA	4911		GLN B 25		69.341	74.272	1.00 41.42	0
MOTA	4912	NE2	GLN B 25	0 -3.333	70.883	74.014	1.00 50.95	N
ATOM	4913	N	GLU B 25	0.611	74.649	72.823	1.00 60.83	N
MOTA	4914	CA	GLU B 25		75.734	71.855	1.00 66.60	С
MOTA	4915	С	GLU B 25		75.992	71.385	1.00 66.06	С
HOTA	4916	Ō	GLU B 25		75.908	70.197	1.00 72.41	0
MOTA	4917	СВ	GLU B 25		77.030	72.459	1.00 77.84	С
MOTA	4918	ĊĞ	GLU B 25		77.224	72.296	1.00 87.92	Ċ
MOTA	4919	CD	GLU B 25		76.123	72.950	1.00 97.98	č
ATOM	4920		GLU B 25		74.957	72.516	1.00102.31	ŏ
MOTA	4921		GLU B 25		76.421	73.900	1.00105.99	. ŏ
MOTA	4922	N	ARG B 25		76.287	72.326	1.00 61.86	N
MOTA	4923	CA	ARG B 25		76.595	72.005	1.00 63.12	Ċ
MOTA	4924	C	ARG B 25		75.413	71.704	1.00 59.63	č
MOTA	4925	Ö			75.483	70.789	1.00 65.66	0
			ARG B 25		77.386	73.138	1.00 05.00	c
MOTA	4925	CB	ARG B 25					
MOTA	4927	CG	ARG B 25	2 4.302	78.659	73.506	1.00 82.92	С

MOTA	4928	CD	ARG 1	B 252	5.048	79.344	74.624	1.00 92.51	С
MOTA	4929	NE		B 252	4.238	80.392	75.228	1.00106.07	Ñ
	4930	CZ		B 252	3.073	80.182	75.837	1.00111.28	Ċ
ATOM							75.926		
MOTA	4931		ARG I		2.576	78.955		1.00112.64	N
MOTA	4932	NH2	ARG		2.402	81.201	76.356	1.00118.84	N
MOTA	4933	N		B 253	5.134	74.344	72.466	1.00 51.23	N
MOTA	4934	CA		B 253	6.014	73.206	72.278	1.00 46.86	С
MOTA	4935	С	ILE !	B 253	5.591	72.105	71.322	1.00 52.26	С
MOTA	4936	0	ILE I	B 253	6.290	71.826	70.352	1.00 54.80	0
ATOM	4937	CB	ILE I	B 253	6.332	72.564	73.621	1.00 37.51	С
ATOM	4938		ILE		5.037	72.266	74.368	1.00 35.63	č
ATOM	4939		ILE		7.210	73.491	74.442	1.00 35.75	č
			ILE		5.259	71.630	75.708	1.00 50.20	č
ATOM	4940	CD1							
ATOM	4941	N		B 254	4.456	71.475	71.601	1.00 57.96	N
ATOM	4942	CA		B 254	3.944	70.370	70.784	1.00 63.04	c
ATOM	4943	С		B 254	4.249	70.475	69.294	1.00 62.84	Ç
ATOM	4944	0		B 254	4.413	69.464	68.603	1.00 62.31	0
MOTA	4945	СВ	VAL	B 254	2.416	70.232	70.927	1.00 63.66	С
ATOM	4946	CG1	VAL	B 254	1.709	71.199	69.963	1.00 71.38	С
MOTA	4947		VAL I		2.004	68.796	70.665	1.00 62.89	С
ATOM	4948	N		B 255	4.326	71.711	68.815	1.00 64.03	N
MOTA	4949	CA		B 255	4.576	72.011	67.413	1.00 66.53	Ċ
ATOM	4950	č		B 255	6.011	71.803	66.911	1.00 63.06	č
							66.012	1.00 65.92	Ö
MOTA	4951	O		B 255	6.245	71.002			Š
MOTA	4952	CB		B 255	4.152	73.449	67.144	1.00 76.95	C
MOTA	4953	CG		B 255	3.518	73.614	65.798	1.00 84.76	c
MOTA	4954		ASP		3.320	74.769	65.366	1.00 92.91	0
MOTA	4955	OD2	ASP		3.210	72.578	65.180	1.00 84.06	0
ATOM	4956	N	VAL	В 256	6.959	72.534	67.491	1.00 55.56	N
ATOM	4957	CA	VAL	B 256	8.368	72.446	67.105	1.00 42.48	С
ATOM	4958	С	VAL	B 256	8.983	71.059	67.301	1.00 41.65	С
MOTA	4959	0		B 256	10.195	70.883	67.195	1.00 36.11	0
ATOM	4960	ČВ		B 256	9.206	73.466	67.898	1.00 39.75	С
ATOM	4961		VAL		8.994	74.864	67.336	1.00 46.21	c c
ATOM	4962		VAL		8.806	73.427	69.350	1.00 37.08	č
ATOM	4963	N		B 257	8.145	70.074	67.585	1.00 45 55	N
					8.613	68.715	67.791	1.00 46.48	č
ATOM	4964	CA		B 257					č
ATOM	4965	C		B 257	8.669	67.932	66.482	1.00 45.47	
ATOM	4966	0_		B 257	7.769	68.024	65.651	1.00 45.44	0
MOTA	4967	CB		B 257	7.704	68.014	68.766	1.00 47.89	C
ATOM	4968	N		B 258	9.725	67.147	66.311	1.00 40.90	N
ATOM	4969	CA	GLY :	B 258	9.878	66.357	65.105	1.00 43.33	С
MOTA	4970	С	GLY :	B 258	11.314	65.889	64.999	1.00 47.01	С
MOTA	4971	0	GLY :	B 258	12.145	66.293	65.809	1.00 49.36	0
ATOM	4972	N		B 259	11.646	65.045	64.013	1.00 47.91	N
ATOM	4973	CA		B 259	13.002	64.527	63.818	1.00 51.95	С
ATOM	4974	c		B 259	14.115	65.546	64.022	1.00 51.79	Č
	4975	ŏ		B 259	14.022	66.681	63.556	1.00 51.46	ŏ
ATOM									č
ATOM	4976	CB		B 259	12.949	64.002	62.399	1.00 51.34	Č
ATOM	4977	CG		В 259	11.592	63.428	62.349	1.00 52.80	C
ATOM	4978	CD		B 259	10.742	64.505	62.988	1.00 48.81	C
ATOM	4979	N		B 260	15.167	65.129	64.721	1.00 48.65	N
ATOM	4980	CA		B 260	16.278	66.019	64.975	1.00 43.90	C
MOTA	4981	С	GLY	B 260	16.125	66.724	66.306	1.00 42.81	С
MOTA	4982	0	GLY	B 260	17.087	66.837	67.057	1.00 47.41	0
MOTA	4983	N	GLY	B 261	14.916	67.197	66.601	1.00 37.57	N
ATOM	4984	CA		B 261	14.666	67.895	67.858	1.00 40.11	С
MOTA	4985	С	GLY	B 261	13.399	67.464	68.585	1.00 40.00	С
ATOM	4986	ŏ		В 261	12.316	67.446	68.004	1.00 40.66	0
ATOM	4987	N		B 262	13.520	67.135	69.866	1.00 35.86	N
ATOM	4988	CA		B 262	12.359	66.683	70.622	1.00 34.24	С
MOTA	4989	C		B 262	12.133	67.402	71.937	1.00 31.66	č
ATOM	4990	ò		B 262	13.048	67.996	72.510	1.00 28.45	ŏ
						65.199	70.951	1.00 28.43	č
MOTA	4991	CB		B 262	12.482				č
MOTA	4992	CG		B 262	12.942	64.349	69.828	1.00 30.95	c
MOTA	4993		TRP		14.204	63.853	69.630	1.00 31.59	Č
ATOM	4994		TRP		12.142	63.849	68.757	1.00 32.51	C
MOTA	4995		TRP		14.231	63.069	68.506	1.00 31.69	N
MOTA	4996		TRP		12.977	63.050	67.951	1.00 30.51	C
MOTA	4997		TRP		10.795	63.993	68.403	1.00 37.67	Č
MOTA	4998	CZ2	TRP	B 262	12.507	62.399	66.806	1.00 38.08	Č
ATOM	4999		TRP		10.328	63.342	67.262	1.00 36.12	С
MOTA	5000		TRP		11.182	62.555	66.481	1.00 38.79	Ċ
ATOM	5001	N		B 263	10.897	67.330	72.420	1.00 27.62	N
ATOM	5002	CA		B 263	10.553	67.916	73.706	1.00 29.78	С
ATOM	5003	c		B 263	10.881	66.844	74.721	1.00 30.61	Č
ATOM	5004	õ		B 263	10.416	65.707	74.587	1.00 34.51	ŏ
MOTA	5005	ČВ		B 263	9.070	68.252	73.766	1.00 27.54	č
ATOM	5005	CG		B 263	8.796	69.689	73.400	1.00 18.61	č
MOTA						70.599	73.949	1.00 19.50	o
	5007 5008			B 263	9.417	69.910	72.484		N
MOTA	5008	NUZ	NON	B 263	7.861	05.510	,	1.00 3.57	N

ATOM	5009	N	ASP	R	264	11.680	62 200	75.727	1 00	29.39	N
	5010						67.200				
ATOM		CA	ASP			12.107	66.241	76.744		33.04	C
ATOM	5011	C	ASP			11.641	66.514	78.178		23.85	С
MOTA	5012	0	ASP	В	264	12.137	67.425	78.838	1.00	16.32	0
MOTA	5013	CB	ASP	В	264	13.635	66.115	76.658	1.00	38.21	С
ATOM	5014	CG	ASP	В	264	14.274	65.627	77.941	1.00	44.50	С
ATOM	5015		ASP			13.840	64.596	78.506		43.89	ō
	5016		ASP							44.94	
ATOM						15.244	66.288	78.373			0
MOTA	5017	N	PRO			10.677	65.701	78.671	-	16.68	N
MOTA	5018	CA	PRO	В	265	10.021	65.698	79.994	1.00	23.78	С
MOTA	5019	С	PRO	В	265	10.999	65.414	81.123	1.00	31.97	С
MOTA	5020	0	PRO	В	265	11.084	66.150	82.112	1.00	36.28	0
MOTA	5021	CB	PRO			8.992	64.569	79.872		15.47	Ċ
ATOM	5022	CG	PRO			8.702	64.519	78.401		17.28	, č
	5023										
MOTA		CD	PRO			10.077	64.660	77.819		19.34	Ċ
MOTA	5024	N	ASP			11.699	64.298	80.953		31.98	N
MOTA	5025	ÇA	ASP			12.719	63.814	81.869	1.00	32.87	С
MOTA	5026	C	ASP	В	266	12.789	62.291	81.881	1.00	37.73	С
MOTA	5027	0	ASP	В	266	12.058	61.599	81.153	1.00	33.38	0
MOTA	5028	СВ			266	12.514	64.327	83.295		32.08	Č
	5029	CG			266			83.963		35.35	č
ATOM						13.831	64.658				
MOTA	5030		ASP			14.861	64.131	83.472		19.67	0
MOTA	5031				266	13.843	65.419	84.963		48.42	0
ATOM	5032	N	MET	В	267	13.680	61.777	82.718	1.00	40.95	N
MOTA	5033	CA	MET	В	267	13.886	60.348	82.830	1.00	36.87	С
MOTA	5034	С	MET	В	267	12.617	59.566	83.150	1.00	35.46	С
ATOM	5035	Õ			267	11.600	60.131	83.559		33.12	Ō
ATOM	5036	ČВ	MET			14.950	60.093	83.889		33.99	č
											Č
ATOM	5037	CG	MET			16.236	60.849	83.611		37.20	C
MOTA	5038	SD	MET			17.220	61.194	85.089		52.40	S
MOTA	5039	CE	MET			16.578	62.777	85.531		54.81	C
MOTA	5040	N	LEU	В	268	12.692	58.258	82.925	1.00	28.80	N
ATOM	5041	CA	LEU	В	268	11.602	57.334	83.203	1.00	20.10	С
MOTA	5042	С	LEU	В	268	11.910	56.720	84.571		25.74	С
ATOM	5043	ō	LEU			12.890	55.985	84.730		34.41	ō
ATOM	5044	СВ	LEU			11.537	56.234	82.134	1.00	3.31	č
-	-										
MOTA	5045	CG	LEU			10.921	56.641	80.795		10.00	C
MOTA	5046		LEU			10.884	55.464	79.832		16.37	С
MOTA	5047	CD2	LEU	В	268	9.507	57.143	81.040	1.00	11.46	С
ATOM	5048	N	VAL	В	269	11.079	57.032	85.560	1.00	25.36	N
ATOM	5049	CA	VAL	В	269	11.289	56.527	86.900	1.00	32.25	С
ATOM	5050	С	VAL	В	269	10.592	55.199	87.161	1.00	29.26	С
ATOM	5051	ō	VAL			10.437	54.778	88.305		29.53	Ō
ATOM	5052	CB	VAL			10.815	57.546	87.914		41.96	Č
ATOM	5053		VAL			11.434	58.895	87.600		46.38	č
ATOM	5054		VAL			9.316	57.633	87.884		49.99	č
ATOM	5055	N	ILE			10.164	54.545	86.091		25.36	Ŋ
MOTA	5056	CA	ILE			9.500	53.247	86.186		28.24	C
MOTA	5057	C	ILE			10.525	52.188	86.593		27.45	C
ATOM	5058	0	ILE			11.608	52.100	86.012		31.99	0
ATOM	5059	CB	ILE	В	270	8.880	52.849	84.825		30.74	С
ATOM	5060	CG1	ILE	В	270	7.737	53.805	84.470	1.00	41.38	C
ATOM	5061	CG2	ILE	В	270	8.381	51.429	84.873	1.00	31.73	С
ATOM	5062		ILE			7.289	53.733	83.016	1.00	46.12	С
ATOM	5063	N	GLY			10.192	51.382	87.592		25.49	N
ATOM	5064	CA	GLY			11.124	50.355	88.022		25.99	Ċ
							50.663	89.385			č
MOTA	5065	Ç	GLY			11.692				30.96	
MOTA	5066	0	GLY			12.432	49.863	89.955		32.97	0
ATOM	5067	N	ASN			11.344	51.845	89.885		35.11	N
ATOM	5068	CA	ASN	В	272	11.770	52.307	91.196	1.00	41.44	С
ATOM	5069	С	ASN	В	272	10.708	51.959	92.227	1.00	43.88	С
MOTA	5070	0	ASN			10.193	50.846	92.226	1.00	50.40	0
ATOM	5071	СВ	ASN			12.012	53.809	91.180		47.76	С
MOTA	5072	ĊĞ	ASN			13.327	54.166	90.558		52.95	Č
ATOM	5073		ASN			13.674	53.664	89.489		61.78	ŏ
								91.218		49.92	N
ATOM	5074					14.073	55.041				
ATOM	5075	N	PHE			10.345	52.914	93.077		40.92	N
ATOM	5076	CA	PHE			9.374	52.644	94.130		45.10	c
ATOM	5077	C	PHE			8.260	53.651	94.287		50.43	. с
ATOM	5078	0	PHE			7.190	53.313	94.775		55.97	0
ATOM	5079	CB	PHE			10.091	52.517	95.478		48.93	c c
MOTA	5080	CG	PHE	В	273	11.593	52.623	95.382	1.00	50.45	С
MOTA	5081		PHE			12.403	51.634	95.920		48.08	С
ATOM	5082		PHE			12.198	53.698	94.728		52.55	Ċ
ATOM	5083		PHE			13.790	51.704	95.808		50.98	С
ATOM	5084		PHE			13.586	53.778	94.608		61.31	č
ATOM	5085	CZ	PHE			14.382	52.776	95.149		59.14	č
ATOM	5086	N	GLY			8.513	54.888	93.889		46.82	N
ATOM	5087	CA	GLY			7.509	55.925	94.040		35.92	č
ATOM	5088	c	GLY			6.213	55.756	93.269		31.72	č
ATOM	5089	ŏ	GLY			5.185	56.352	93.633		33.90	Ö
	5-55	•	201	ی	~ / 7	5.105	50.552			JJ. 30	U

MOTA	5090	N	LEU		275	6.239	54.941	92.218	1 00	20 07	N.
ATOM	5091	CA								28.97	N
	5092		LEU		275	5.038	54.744	91.419		26.12	C
ATOM		C	LEU		275	4.311	53.425	91.608		28.74	C
ATOM	5093	0	LEU		275	4.931	52.372	91.748		31.57	0
ATOM	5094	CB	LEU			5.369	54.930	89.945		26.02	C
ATOM	5095	CG	LEU			5.958	56.304	89.620		23.75	Č
MOTA	5096				275	5.811	56.551	88.130		28.23	Ċ
ATOM	5097		LEU			5.231	57.396	90.414		22.80	С
ATOM	5098	N	SER			2.986	53.498	91.630		28.06	N
MOTA	5099	CA	SER			2.182	52.302	91.770		36.79	С
ATOM	5100	С	SER			2.153	51.726	90.367		40.22	c c
MOTA	5101	0	SER			2.698	52.314	89.440		38.89	0
ATOM	5102	CB	SER			0.766	52.652	92.181	1.00	40.24	C 0
MOTA	5103	OG	SER			0.083	53.229	91.078	1.00	45.11	0
MOTA	5104	N	TRP			1.493	50.589	90.206		43.13	N
ATOM	5105	CA	TRP			1.422	49.965	88.907		39.95	c c
ATOM	5106	С	TRP			0.660	50.820	87.936		36.27	С
MOTA	5107	0	TRP			1.149	51.135	86.845		35.96	0
ATOM	5108	CB	TRP			0.732	48.612	88.972		46.97	0 0 0
ATOM	5109	CG	TRP		277	0.617	48.018	87.607	1.00	46.70	С
MOTA	5110		TRP		277	-0.530	47.728	86.928	1.00	46.98	С
ATOM	5111	CD2	TRP		277	1.701	47.695	86.725	1.00	48.84	С
ATOM	5112	NE1	TRP		277	-0.230	47.244	85.674	1.00	45.37	N
ATOM	5113	CE2	TRP	В	277	1.132	47.214	85.523	1.00	48.55	С
MOTA	5114	CE3	TRP	В	277	3.099	47.768	86.835	1.00	49.30	C C
ATOM	5115	CZ2	TRP	В	277	1.912	46.806	84.435	1.00	44.51	С
MOTA	5116	CZ3	TRP	В	277	3.874	47.365	85.759	1.00	45.41	С
ATOM	5117	CH2	TRP	В	277	3.276	46.889	84.570	1.00	42.60	С
MOTA	5118	N	ASN	В	278	-0.556	51.177	88.314	1.00	32.20	N
ATOM	5119	CA	ASN	В	278	-1.359	51.984	87.423	1.00	31.29	С
MOTA	5120	С	ASN	В	278	-0.672	53.268	87.060	1.00	31.61	С
ATOM	5121	0	ASN	В	278	-0.885	53.804	85.975	1.00	32.14	0
MOTA	5122	CB	ASN	В	278	-2.693	52.278	88.059	1.00	36.76	С
MOTA	5123	CG	ASN	В	278	-3.697	51.231	87.735	1.00	37.14	С
MOTA	5124	OD1	ASN	В	278	-4.181	51.161	86.604	1.00	30.93	0
ATOM	5125	ND2	ASN	В	278	-4.006	50.379	88.714	1.00	42.27	N
MOTA	5126	N	GLN	В	279	0.171	53.742	87.970	1.00	32.31	N
MOTA	5127	CA	GLN	В	279	0.897	54.978	87.759	1.00	31.16	С
MOTA	5128	С	GLN	В	279	2.053	54.829	86.775	1.00	34.55	С
MOTA	5129	0	GLN	В	279	2.360	55.757	86.035	1.00	31.95	0
ATOM	5130	CB	GLN	В	279	1.390	55.506	89.099	1.00	19.15	С
ATOM	5131	CG	GLN	В	279	0.288	56.135	89.909	1.00	3.31	С
MOTA	5132	CD	GLN	В	279	0.619	56.185	91.367	1.00	4.33	С
MOTA	5133	OE1	GLN	В	279	1.751	56.473	91.743	1.00	20.32	0
MOTA	5134	NE2	GLN	В	279	-0.371	55.907	92.211	1.00	9.62	N
MOTA	5135	N	GLN	В	280	2.682	53.659	86.757	1.00	35.28	N
MOTA	5136	CA	GLN	В	280	3.795	53.414	85.851	1.00	28.21	С
MOTA	5137	С	GLN	В	280	3.335	53.340	84.390	1.00	33.39	С
MOTA	5138	0	GLN	В	280	3.913	53.998	83.513	1.00	29.04	0
MOTA	5139	CB	GLN	В	280	4.517	52.119	86.232	1.00	19.60	С
MOTA	5140	CG	GLN	В	280	5.061	52.098	87.637		25.07	С
ATOM	5141	CD	GLN	В	280	5.960	50.915	87.897	1.00	33.96	С
ATOM	5142	OE1	GLN	В	280	7.058	50.830	87.351	1.00	39.59	0
MOTA	5143	NE2	GLN	В	280	5.498	49.987	88.727		35.05	N
MOTA	5144	N	VAL			2.300	52.550	84.118		33.52	N
ATOM	5145	CA	VAL	В	281	1.822	52.445	82.744		33.85	С
MOTA	5146	С	VAL		281	1.543	53.841	82.219		32.53	Č
MOTA	5147	0	VAL			1.828	54.158	81.072		34.07	Ō
ATOM	5148	CB	VAL			0.526	51.599	82.638		31.50	Č
ATOM	5149		VAL			0.697	50.324	83.426		32.91	C
MOTA	5150	CG2	VAL			-0.682	52.392	83.126		33.47	C
MOTA	5151	N			282	0.992	54.677	83.086		23.34	N
ATOM	5152	CA	THR			0.664	56.036	82.714		12.70	C
ATOM	5153	С	THR			1.873	56.762	82.134		11.31	Č
ATOM	5154	0	THR			1.831	57.183	80.981		17.88	0
MOTA	5155	CB	THR			0.135	56.826	83.920		15.31	c
ATOM	5156		THR			-0.916	56.093	84.564		16.34	0
MOTA	5157		THR			-0.406	58.160	83.465		17.32	C
MOTA	5158	N	GLN			2.948	56.898	82.916	1.00	4.99	N
ATOM	5159	CA	GLN			4.148	57.593	82.428		10.41	c
MOTA	5160	C	GLN			4.606	57.030	81.084		13.30	c
MOTA	5161	0	GLN			4.811	57.772	80.126		15.31	0
ATOM	5162	CB	GLN			5.327	57.499	83.418	1.00	3.31	c
ATOM	5163	CG	GLN			6.612	58.139	82.837		23.14	c
MOTA	5164	CD	GLN			7.843	58.027	83.732		32.77	c
ATOM	5165		GLN			8.285	56.931	84.071		34.41	0
ATOM	5166		GLN			8.409	59.170	84.103 81.028			N N
ATOM	5167 5168	N	MET			4.779	55.714 55.055	79.803		15.81	N C
ATOM	5168 5169	CA	MET			5.194	55.376	78.667		14.55 11.07	Ċ
MOTA MOTA	5169 5170	C O	MET MET			4.225 4.640	55.794	77.596	1.00	5.42	o
	~ 0	~	• • • •	•	204	4.040			4.00	J. 76	U

ATOM	5171	СВ	MET E	3 284	5.238	53.546	80.022	1.00 13.69	(С
ATOM	5172	ĊĠ	MET E		5.767	52.755	78.844	1.00 8.27		č
ATOM	5173	SD	MET E		7.559		78.676	1.00 21.12		s
						52.899			3	2
ATOM	5174	CE	MET E		7.661	53.878	77.067	1.00 26.82	(
MOTA	5175	N	ALA E		2.934	55.171	78.899	1.00 9.54	ì	
MOTA	5176	CA	ALA E	3 285	1.936	55.446	77.878	1.00 12.00	(С
ATOM	5177	С	ALA E	285	2.054	56.872	77.374	1.00 13.36	(2
ATOM	5178	0	ALA E	285	2.098	57.112	76.160	1.00 17.10		ō
ATOM	5179	ČВ	ALA E		0.546	55.218	78.428	1.00 23.30	5	
ATOM	5180	N	LEU E		2.113	57.825	78.296	1.00 12.23	í	
	5181									
ATOM		CA	LEU E		2.206	59.216	77.887	1.00 14.82	Q	_
ATOM	5182	C	LEU E		3.544	59.671	77.306	1.00 18.25	(C
ATOM	5183	0	LEU E		3.551	60.513	76.410	1.00 29.59	()
MOTA	5184	CB	LEU E		1.740	60.129	79.018	1.00 19.13	(2
ATOM	5185	CG	LEU E	286	0.208	60.174	78.942	1.00 12.90	(2
ATOM	5186	CD1	LEU E	286	-0.385	60.212	80.316	1.00 24.27	(C
ATOM	5187	CD2	LEU E	286	-0.233	61.371	78.145	1.00 7.95	(ċ
ATOM	5188	N	TRP B		4.671	59.138	77.769	1.00 16.94	1	Ň
ATOM	5189	CA	TRP E		5.924	59.560	77.160	1.00 25.08	·	ř
ATOM	5190	c	TRP B		5.850	59.156	75.694	1.00 30.58	č	~
ATOM)	-
	5191	0	TRP B		6.353	59.855	74.810	1.00 37.20	(
ATOM	5192	CB	TRP B		7.121	58.894	77.812	1.00 19.43	Ç	Ľ
ATOM	5193	CG	TRP B		7.782	59.744	78.855	1.00 27.34	(2
ATOM	5194	CD1	TRP B	287	9.125	59.961	79.004	1.00 40.95	(С
MOTA	5195	CD2	TRP B	287	7.145	60.463	79.916	1.00 20.62	(0
ATOM	5196	NE1	TRP B	287	9.370	60.763	80.099	1.00 28.11	f	N
ATOM	5197	CE2	TRP B	287	8.173	61.080	80.681	1.00 18.44		С
ATOM	5198	CE3	TRP B		5.814	60.631	80.313	1.00 19.29	. (Ċ
ATOM	5199	CZ2			7.908	61.871	81.794	1.00 22.11	č	~
ATOM	5200	CZ3			5.552	61.417	81.421	1.00 33.41	ò	~
			TRP E					1.00 28.12	Č	~
ATOM	5201				6.596	62.022	82.156			
ATOM	5202	N	ALA B		5.204	58.024	75.441	1.00 27.82	1	N
MOTA	5203	CA	ALA B		5.043	57.531	74.084	1.00 26.69	(J
MOTA	5204	С	ALA B		4.188	58.509	73.293	1.00 25.25	(2
MOTA	5205	0	ALA E	288	4.467	58.794	72.124	1.00 19.52	(
MOTA	5206	CB	ALA B	288	4.388	56.167	74.104	1.00 33.43	(С
ATOM	5207	N	ILE B	289	3.142	59.025	73.934	1.00 20.43	ı	N
ATOM	5208	CA	ILE B	289	2.258	59.975	73.266	1.00 23.46	(С
ATOM	5209	C	ILE B		3.002	61.256	72.960	1.00 30.21	Ċ	ē
ATOM	5210	ō	ILE B		2.797	61.857	71.907	1.00 39.56	Ċ	ā
ATOM	5211	ČВ	ILE B		1.039	60.348	74.125	1.00 20.26	ò	ř
ATOM	5212		ILE B		0.093	59.150	74.233	1.00 20.20	ò	~
									Č	~
ATOM	5213		ILE B		0.305	61.528	73.488	1.00 17.24	,	=
MOTA	5214		ILE B		-0.599	58.824	72.916	1.00 16.19	(
MOTA	5215	N	MET B		3.871	61.667	73.882	1.00 23.96	1	
ATOM	5216	CA	MET B		4.62B	62.900	73.710	1.00 20.64	(¢
ATOM	5217	С	MET B	290	6.004	62.752	73.088	1.00 22.98	C	С
MOTA	5218	0	MET B	290	6.933	63.463	73.509	1.00 29.05	(0
MOTA	5219	CB	MET B	290	4.815	63.582	75.047	1.00 22.08	(С
ATOM	5220	CG	MET B	290	3.566	63.737	75.855	1.00 21.11	(C
ATOM	5221	SD	MET B	290	4.061	64.589	77.350	1.00 19.71	9	s
ATOM	5222	CE	MET B		4.643	63.133	78.403	1.00 3.31	9	Ċ
ATOM	5223	N	ALA B		6.135	61.863	72.099	1.00 23.81	ì	
ATOM	5224	CA	ALA B		7.415	61.638	71.447	1.00 25.68	·	
ATOM	5225	c	ALA B		8.488	62.261	72.329	1.00 23.85	č	
ATOM	5226	ŏ	ALA B		9.094		71.987	1.00 26.09		Ö
						63.282				
ATOM	5227 5228	CB	ALA B		7.420	62.278	70.086	1.00 28.53	(N
ATOM		N	ALA B		8.685	61.664	73.497			
MOTA	5229	CA	ALA B		9.674			1.00 25.88	9	
ATOM	5230	Ċ	ALA B		10.872	61.224	74.482	1.00 22.90		С
ATOM	5231	0	ALA B		10.742	60.030	74.199	1.00 18.54		0
ATOM	5232	СВ	ALA B		9.054	62.293	75.817	1.00 31.58		С
ATOM	5233	N	PRO B	293	12.060	61.749	74.837	1.00 22.52		Ν
ATOM	5234	CA	PRO B	293	13.217	60.856	74.893	1.00 28.95	(С
MOTA	5235	С	PRO B		12.964	59.820	75.994	1.00 33.22	(С
ATOM	5236	0	PRO B	293	12.453	60.151	77.066	1.00 37.99	(0
ATOM	5237	СB	PRO B		14.379	61.802	75.237	1.00 31.26	Č	С
MOTA	5238	CG	PRO B		13.911	63.147	74.783	1.00 35.10	à	C
ATOM	5239	CD	PRO B		12.453	63.130	75.179	1.00 29.37	à	c
ATOM	5240	N	LEU B		13.315	58.570	75.723	1.00 33.61	ì	N
ATOM	5241	CA	LEU B		13.121	57.511	76.696	1.00 30.85	;	ċ
ATOM	5242	C	LEU B			57.213	77.455	1.00 30.83	,	c
					14.393	56.524	76.950)	č
ATOM	5243	0	LEU B		15.291			1.00 26.27	9	0
MOTA	5244	CB	LEU B		12.650	56.242	76.007	1.00 37.34	9	-
MOTA	5245	CG	LEU B		11.398	56.505	75.184	1.00 35.26	9	_
ATOM	5246		LEU B		11.000	55.233	74.453	1.00 42.55	(0000
	5247	CD2	LEU B		10.278	57.009	76.098	1.00 26.36	(ċ
ATOM						- 7771	78.669			
MOTA	5248	N	PHE B		14.475	57.743		1.00 30.92	1	N
MOTA MOTA	5248 5249	CA	PHE B	295	15.632	57.502	79.506	1.00 34.03	(С
MOTA MOTA MOTA	5248 5249 5250	CA C	PHE B	295 295	15.632 15.218	57.502 56.972	79.506 80.858	1.00 34.03 1.00 34.10	(c
MOTA MOTA	5248 5249	CA	PHE B	295 295	15.632	57.502	79.506	1.00 34.03	(С

ATOM	5252	CB	PHE	R	295	16.448	58.774	79.687	1 00	36.16	С
MOTA	5253	CG	PHE		295	17.311	59.079	78.527	1.00	30.56	С
ATOM	5254	CD1	PHE	В	295	16.749	59.300	77.286	1.00	34.14	С
ATOM	5255	CD2		R	295	18.688	59.091	78.656	1 00	26.11	С
ATOM	5256	CEl	PHE	В	295	17.544	59.526	76.181	1.00	38.29	С
ATOM	5257	CE2	PHE	В	295	19.496	59.316	77.562	1.00	35.19	С
ATOM	5258	CZ	PHE		295	18.924	59.534	76.318		36.95	C
ATOM	5259	N	MET		296	15.603	55.733	81.128	1.00	22.48	N
ATOM	5260	CA	MET	В	296	15.280	55.140	82.401	1.00	21.21	С
ATOM	5261		MET		296	16.238		83.432	1.00	8.44	č
		Ç					55.715				
ATOM	5262	0	MET	В	296	17.267	56.304	83.100	1.00	12.07	0
ATOM	5263	CB	MET	В	296	15.458	53.625	82.329	1.00	29.96	С
		CG			296	14.637	52.943	81.257		36.98	č
ATOM	5264		MET								c s c
ATOM	5265	SD	MET	В	296	15.077	51.204	81.136	1.00	38.86	S
ATOM	5266	CE	MET	В	296	16.504	51.292	80.091	1.00	33.37	c
ATOM	5267	N			297	15.870	55.559	84.688	1.00	3.31	N
ATOM	5268	CA	SER	В	297	16.699	55.986	85.791	1.00	8.77	С
ATOM	5269	С	SER	В	297	16.290	54.970	86.822	1.00	18.70	С
ATOM	5270	Õ	SER		297	15.508	55.254	87.724		22.71	Ō
ATOM	5271	СВ	SER	В	297	16.338	57.395	86.259	1.00	14.75	С
MOTA	5272	OG	SER	В	297	17.177	57.802	87.337	1.00	8.66	0
ATOM	5273	N	ASN		298	16.798	53.764	86.650		22.61	N
ATOM	5274	CA	ASN	В	298	16.484	52.687	87.558		29.60	С
ATOM	5275	С	ASN	В	298	17.692	51.780	87.645	1.00	34.27	С
ATOM	5276	Ō	ASN		298	18.615	51.887	86.832		28.75	0
MOTA	5277	СВ	ASN	В	298	15.276	51.912	87.030		32.96	С
ATOM	5278	CG	ASN	В	298	15.341	51.698	85.535	1.00	38.86	C
MOTA	5279		ASN		298	16.273	51.066	85.024	1 00	39.71	0
MOTA	5280	ND2			298	14.356	52.234	84.816		41.15	N
MOTA	5281	N	ASP	В	299	17.695	50.904	88.641	1.00	38.90	N
MOTA	5282	CA	ASP			18.779	49.960	88.772		39.76	С
MOTA	5283	С	ASP		299	18.326	48.711	88.014		42.94	С
MOTA	5284	0	ASP	В	299	17.504	47.951	88.521	1.00	56.20	0
MOTA	5285	СВ	ASP	R	299	19.015	49.622	90.232		43.59	С
MOTA	5286	CG	ASP			20.187	48.700	90.415		61.39	Ç
ATOM	5287	OD1	ASP	В	299	20.475	47.933	89.478	1.00	69.62	0
MOTA	5288	002	ASP	R	299	20.814	48.721	91.494	1.00	72.12	0
											N
MOTA	5289	N	LEU		300	18.858	48.512	86.807		37.42	
MOTA	5290	CA	LEU	В	300	18.500	47.367	85.968	1.00	37.23	С
MOTA	5291	С	LEU	R	300	18.888	46.014	86.576	1.00	39.88	С
	5292	ŏ			300	18.591	44.963	86.005		46.92	Õ
ATOM			LEU								
ATOM	5293	CB	LEU	В	300	19.135	47.500	84.571	1.00	33.44	С
ATOM	5294	CG	LEU	В	300	18.767	48.687	83.670	1.00	42.19	С
						19.097	49.983	84.378		49.28	Ċ
MOTA	5295		LEU		300						
ATOM	5296	CD2	LEU	В	300	19.538	48.609	82.354	1.00	41.83	. с
ATOM	5297	N	ARG	В	301	19.543	46.040	87.736	1.00	36.03	N
MOTA	5298	CA	ARG			19.965	44.822	88.438		43.28	С
											č
MOTA	5299	C	ARG	В	301	18.796	44.373	89.297		50.61	С
ATOM	5300	0	ARG	В	301	18.327	43.237	89.210	1.00	53.65	0
ATOM	5301	CB	ARG			21.149	45.137	89.346	1.00	43.12	С
ATOM	5302	CG	ARG		301	22.253	45.888	88.624		46.62	C
ATOM	5303	CD	ARG	В	301	23.340	46.421	89.553	1.00	56.63	С
ATOM	5304	NE	ARG	R	301	22.939	47.621	90.285	1.00	58.70	N
						23.778					
MOTA	5305	CZ	ARG		301		48.381	90.980		63.45	C
ATOM	5306	NH1	ARG	В	301	25.064	48.074	91.041	1.00	64.54	N
ATOM	5307	NH2			301	23.332	49.447	91.619	1.00	72.40	N
MOTA	5308	N	HIS		302	18.343	45.304	90.128		56.54	N
MOTA	5309	CA	HIS			17.229	45.082	91.021		64.34	C
MOTA	5310	С	HIS	В	302	16.012	45.816	90.469	1.00	60.12	С
ATOM	5311	0	HIS			15.606	46.864	90.983	1.00	64.27	0
	5312					17.564	45.594	92.425		73.45	č
ATOM		СВ	HIS								č
ATOM	5313	CG	HIS			18.838	45.037	92.984		85.14	С
ATOM	5314	ND1	HIS	В	302	18.988	43.708	93.314	1.00	91.07	N
ATOM	5315		HIS			20.029	45.625	93.244		91.96	Ċ
											č
MOTA	5316		HIS			20.218	43.499	93.751		94.56	
MOTA	5317	NE2	HIS	В	302	20.870	44.647	93.718		97.45	N
ATOM	5318	N	ILE			15.455	45.269	89.391		52.24	N
							45.837	88.763			Ċ
ATOM	5319	CA	ILE			14.274				42.64	٠
ATOM	5320	С	ILE			13.231	44.745	88.606		45.64	C
MOTA	5321	0	ILE			13.535	43.642	88.143	1.00	43.87	0
ATOM	5322	ČВ	ILE			14.596	46.424	87.374		41.50	č
											_
MOTA	5323		ILE			13.331	47.030	86.769		49.28	C
ATOM	5324	CG2	ILE	В	303	15.139	45.343	86.458	1.00	34.23	С
ATOM	5325	CD1	ILE	Ř	303	13.575	47.812	85.514		50.30	ŗ
											C C N
MOTA	5326	N	SER			12.008	45.057	89.013		46.67	N
ATOM	5327	CA	SER	В	304	10.898	44.119	88.930		48.72	С
ATOM	5328	С	SER			10.760	43.527	87.541	1.00	49.16	С
ATOM	5329	õ	SER			11.070	44.185	86.550		50.82	ñ
								89.306			c c o c
ATOM	5330	СВ	SER			9.607	44.833			49.11	Č
MOTA	5331	OG	SER	В	304	9.765	46.233	89.168		52.40	0
MOTA	5332	N	PRO	В	305	10.304	42.268	87.446	1.00	53.50	N

MOTA	5333	CA	PRO	B 305	10.138	41.632	86.136	1.00 55.43	С
MOTA	5334	C	PRO		8.950	42.309	85.463	1.00 53.13	C
MOTA	5335	0	PRO	B 305	8.975	42.630	84.266	1.00 41.46	0
MOTA	5336	CB	PRO	B 305	9.826	40.178	86.489	1.00 56.22	Ċ
		CG							-
ATOM	5337			B 305	10.401	40.014	87.847	1.00 60.62	С
MOTA	5338	CD	PRO	B 305	10.038	41.305	88.521	1.00 58.74	С
ATOM	5339	N	GLN	B 306	7.909	42.514	86.268	1.00 57.38	N
	5340								
MOTA		CA		B 306	6.691	43.154	85.816	1.00 63.53	С
ATOM	5341	С	GLN	B 306	7.023	44.523	85.238	1.00 62.83	C
ATOM	5342	0	GLN	B 306	6.424	44.946	84.258	1.00 64.21	o
									9
MOTA	5343	CB		B 306	5.703	43.282	86.983	1.00 70.70	С
ATOM	5344	CG	GLN	B 306	6.277	43.885	88.256	1.00 88.06	c
ATOM	5345	CD	GLN	B 306	5.228	44.056	89.338	1.00 98.86	Ċ
ATOM	5346		GLN		4.598	43.089	89.765	1.00108.90	0
MOTA	5347	NE2	GLN	B 306	5.032	45.293	89.788	1.00100.01	N
ATOM	5348	N	A.I.A	B 307	7.992	45.206	85.838	1.00 60.27	N
ATOM	5349	CA		B 307	8.400	46.525	85.368	1.00 52.67	С
ATOM	5350	С	ALA	B 307	9.104	46.388	84.027	1.00 49.37	C
ATOM	5351	0	AI.A	B 307	8.612	46.870	83.009	1.00 47.80	0
	5352	ČВ		B 307					
MOTA					9.328	47.179	86.376	1.00 50.06	С
MOTA	5353	N		B 308	10.260	45.729	84.041	1.00 48.26	N
MOTA	5354	CA	LYS	B 308	11.056	45.509	82.831	1.00 49.41	С
ATOM	5355	C		B 308	10.185	45.131	81.636	1.00 47.85	č
									č
ATOM	5356	0		B 308	10.506	45.464	80.492	1.00 42.82	0
ATOM	5357	CB	LYS :	B 308	12.075	44.388	83.059	1.00 51.52	c
ATOM	5358	ĊG		B 308	12.844	44.012	81.802	1.00 58.09	. č
ATOM	5359	CD		B 308	13.486	42.648	81.907	1.00 65.32	· c
ATOM	5360	CE	LYS	B 308	12.437	41.566	82.032	1.00 72.87	С
MOTA	5361	NZ	LYS	B 308	13.054	40.221	81.974	1.00 73.72	N
ATOM	5362	N		B 309	9.099	44.414	81.910		
								1.00 46.79	N
MOTA	5363	CA		B 309	8.184	43.986	80.864	1.00 43.70	C
ATOM	5364	C	ALA :	B 309	7.609	45.208	80.176	1.00 39.92	c
ATOM	5365	Ó	A F. A	B 309	7.671	45.351	78.952	1.00 40.53	ō
MOTA	5366	CB	ALA		7.071	43.154	81.461	1.00 45.68	С
MOTA	5367	N	LEU	B 310	7.045	46.091	80.986	1.00 36.87	N
ATOM	5368	CA	LEU :	B 310	6.464	47.325	80.491	1.00 32.15	C
	5369	Ċ			7.526				č
ATOM				B 310		48.151	79.771	1.00 30.53	ب
ATOM	5370	0	LEU	B 310	7.392	48.442	78.596	1.00 27.92	0
ATOM	5371	СB	LEU :	B 310	5.892	48.124	81.661	1.00 33.14	С
ATOM	5372	ĊG	LEU		5.357	49.532	81.400	1.00 40.85	Ċ
									_
ATOM	5373		LEU		4.349	49.513	80.252	1.00 52.52	C
MOTA	5374	CD2	LEU :	B 310	4.723	50.071	82.693	1.00 50.61	C
ATOM	5375	N	LEU	B 311	8.584	48.523	80.482	1.00 26.12	N
ATOM	5376	CA	LEU		9.671	49.308	79.910	1.00 25.13	Ċ
									Č
ATOM	5377	С	LEU :		10.113	48.841	78.515	1.00 32.11	С
MOTA	5378	0	LEU :	B 311	10.567	49.649	77.700	1.00 33.23	0
ATOM	5379	СВ		B 311	10.865	49.280	80.864	1.00 12.06	C
ATOM	5380	CG		B 311	10.705	50.239	82.036	1.00 26.57	С
MOTA	5381	CD1	LEU :	B 311	11.473	49.752	83.244	1.00 31.27	С
MOTA	5382	CD2	LEU :	B 311	11.182	51.614	81.598	1.00 17.17	c
ATOM	5383	N	CLN :	B 312	9.972	47.544	78.239	1.00 36.20	N
ATOM	5384	CA	GLN :		10.383	46.972	76.958	1.00 36.10	c
MOTA	5385	С	GLN :	B 312	9.260	46.597	76.002	1.00 42.91	С
ATOM	5386	0	GLN :	B 312	9.535	46.061	74.935	1.00 46.16	0
MOTA	5387	CB		B 312	11.243	45.731	77.198	1.00 34.90	Ċ
MOTA	5388	CG		B 312	12.474	45.966	78.052	1.00 43.65	c
MOTA	5389	CD	GLN		13.431	44.787	78.039	1.00 45.97	С
ATOM	5390	OE1	GLN I	B 312	13.015	43.641	78.168	1.00 51.35	0
ATOM	5391		GLN		14.722	45.066	77.892	1.00 42.69	N
ATOM	5392			B 313	8.008	46.870	76.359	1.00 45.00	N
		N							
ATOM	5393	CA		B 313	6.892	46.527	75.474	1.00 51.81	Č
MOTA	5394	С	ASP 1	B 313	7.108	47.009	74.025	1.00 53.55	С
MOTA	5395	Ō		B 313	6.974	48.202	73.722	1.00 49.29	Ō
MOTA	5396	СВ		B 313	5.576	47.103	76.005	1.00 54.01	č
									Č
MOTA	5397	CG		B 313	4.361	46.603	75.220	1.00 60.77	c
ATOM	5398	OD1	ASP I	B 313	4.414	46.610	73.961	1.00 64.06	0
MOTA	5399		ASP		3.353	46.215	75.857	1.00 53.70	ō
MOTA	5400	N		B 314	7.416	46.062	73.139	1.00 57.01	N
MOTA	5401	CA	LYS I	B 314	7.681	46.344	71.730	1.00 61.78	С
ATOM	5402	С		B 314	6.675	47.266	71.048	1.00 58.40	С
ATOM	5403					48.159	70.294	1.00 60.17	ŏ
		0		B 314	7.058				ō
ATOM	5404	CB	LYS 1		7.740	45.036	70.934	1.00 76.80	С
ATOM	5405	CG	LYS 1	B 314	8.778	44.038	71.422	1.00102.87	С
ATOM	5406	CD		B 314	8.732	42.756	70.587	1.00117.39	č
ATOM	5407	CE				41.776	71.005		č
				B 314	9.822			1.00124.70	
MOTA	5408	NZ	LYS		9.841	40.579	70.115	1.00132.68	N
ATOM	5409	N	ASP I	B 315	5.392	47.032	71.301	1.00 56.81	N
MOTA	5410	CA		B 315	4.317	47.810	70.687	1.00 50.96	ċ
MOTA	5411	c				49.248	71.169		č
				B 315	4.255			1.00 46.39	
ATOM	5412	0		B 315	3.860	50.143	70.412	1.00 41.44	0
MOTA	5413	CB	ASP I	B 315	2.976	47.135	70.961	1.00 54.17	С

ATOM	5414	CG	ASP I	3 315	3.016	45.649	70.699	1.00 60.24	С
ATOM	5415	OD1			3.030	45.253	69.513	1.00 57.63	ō
MOTA	5416	OD2	ASP I	3 3 1 5	3.041	44.880	71.687	1.00 62.09	0
MOTA	5417	N	VAL I		4.634	49.469	72.428	1.00 42.81	N
MOTA	5418	CA	VAL I		4.601	50.812	72.994	1.00 41.35	C
ATOM	5419	C	VAL I		5.838 5.753	51.596 52.778	72.578	1.00 49.57	C
MOTA MOTA	5420 5421	O CB	VAL I		4.488	50.759	72.234 74.535	1.00 56.13 1.00 30.91	0 C
ATOM	5422		VAL I		4.408	52.170	75.117	1.00 37.66	Ċ
MOTA	5423		VAL I		3.241	49.990	74.924	1.00 38.09	č
ATOM	5424	N	ILE E		6.988	50.935	72.598	1.00 52.84	N
MOTA	5425	CA	ILE E		8.221	51.590	72.189	1.00 50.65	С
MOTA	5426	C	ILE E		8.046	52.038	70.747	1.00 51.01	c
ATOM	5427	0	ILE E		8.483 9.403	53.115 50.628	70.355 72.232	1.00 49.49 1.00 47.80	0 C
MOTA MOTA	5428 5429	CB CG1	ILE E		9.421	49.888	73.568	1.00 47.80	Ċ
ATOM	5430	CG2	ILE E		10.695	51.401	72.016	1.00 49.27	č
ATOM	5431		ILE E		10.497	48.824	73.658	1.00 57.21	Ċ
MOTA	5432	N	ALA E	318	7.396	51.184	69.968	1.00 47.41	N
MOTA	5433	CA	ALA E		7.139	51.453	68.569	1.00 47.73	C
MOTA	5434	c	ALA I		6.400 6.787	52.765	68.443	1.00 45.10 1.00 51.89	C C
ATOM ATOM	5435 5436	O CB	ALA I		6.315	53.641 50.331	67.680 67.965	1.00 49.34	Č
ATOM	5437	N	ILE I		5.327	52.910	69.195	1.00 38.46	N
ATOM	5438	CA	ILE I		4.574	54.146	69.123	1.00 35.63	Ċ
MOTA	5439	С	ILE E	3 319	5.474	55.344	69.390	1.00 36.82	С
MOTA	5440	0	ILE I		5.567	56.249	68.574	1.00 41.34	0
ATOM	5441	CB	ILE I		3.407	54.128	70.118	1.00 33.97	c
ATOM ATOM	5442 5443	CG1 CG2	ILE I		2.335. 2.837	53.165 55.531	69.607 70.302	1.00 42.09 1.00 23.48	C
MOTA	5444		ILE I		1.200	52.970	70.559	1.00 54.00	č
ATOM	5445	N	ASN I		6.149	55.349	70.528	1.00 35.81	N
ATOM	5446	CA	ASN I		7.035	56.459	70.859	1.00 36.40	С
MOTA	5447	C	ASN I		8.121	56.649	69.800	1.00 35.02	c
ATOM	5448	0	ASN I		8.548	57.777	69.534	1.00 38.20	0
ATOM ATOM	5449 5450	CB CG	ASN I		7.675 8.791	56.222 57.189	72.232 72.527	1.00 43.77 1.00 50.25	C C
ATOM	5451	ODI	ASN I		9.820	57.183	71.856	1.00 55.90	ō
ATOM	5452		ASN I		8.595	58.031	73.536	1.00 51.06	N
MOTA	5453	N	GLN I		8.553	55.539	69.199	1.00 37.76	N
ATOM	5454	CA	GLN I		9.605	55.542	68.176	1.00 49.96	C
ATOM	5455	c	GLN I		9.075 9.796	55.766 55.571	66.768 65.785	1.00 57.68 1.00 59.07	C 0
ATOM ATOM	5456 5457	O CB	GLN I		10.381	54.217	68.206	1.00 44.90	c
ATOM	5458	CG	GLN I		11.433	54.121	69.288	1.00 46.70	č
ATOM	5459	CD	GLN I		12.465	55.214	69.156	1.00 47.84	С
MOTA	5460	OE1	GLN I		13.001	55.445	68.075	1.00 39.88	0
MOTA	5461	NE2	GLN I		12.748	55.898	70.255	1.00 41.72	N
ATOM	5462 5463	N CA	ASP I		7.811 7.179	56.163 56.415	66.677 65.388	1.00 62.92 1.00 60.53	N C
ATOM ATOM	5464	CV	ASP I		8.128	57.252	64.543	1.00 54.21	č
MOTA	5465	ŏ	ASP I		8.665	58.258	65.007	1.00 50.45	ō
MOTA	5466	CB	ASP I		5.846	57.142	65.592	1.00 63.03	С
MOTA	5467	CG	ASP I		5.023	57.222	64.330	1.00 60.44	C
MOTA	5468 5469		ASP I		4.739	56.161 58.351	63.729 63.954	1.00 51.90 1.00 56.64	0
ATOM ATOM	5470	OD2 N	PRO I		8.340	56.844	63.287	1.00 48.81	N
ATOM	5471	CA	PRO I		9.227	57.517	62.336	1.00 49.20	Ċ
MOTA	5472	С	PRO I		8.723	58.889	61.960	1.00 49.78	C
ATOM	5473	0	PRO I		9.507	59.781	61.661	1.00 50.30	0
ATOM	5474	CB	PRO I		9.210	56.579 56.174	61.147 61.116	1.00 49.51 1.00 54.97	c c
MOTA MOTA	5475 5476	CG CD	PRO I		7.765 7.485	55.866	62.586	1.00 50.18	č
ATOM	5477	N	LEU I		7.405	59.036	61.965	1.00 46.95	N
ATOM	5478	CA	LEU I		6.769	60.290	61.619	1.00 46.62	С
ATOM	5479	Ç	LEU I		7.305	61.438	62.469	1.00 46.44	c
ATOM	5480	0	LEU I		7.764	62.444	61.938	1.00 50.63	0
ATOM ATOM	5481 5482	CB CG	LEU I		5.262 4.419	60.179 60.922	61.809 60.775	1.00 52.20 1.00 54.98	c c
ATOM	5483		LEU I		3.002	61.035	61.284	1.00 53.77	С
ATOM	5484		LEU I		4.991	62.300	60.518	1.00 54.88	С
MOTA	5485	N	GLY I	3 325	7.234	61.302	63.786	1.00 42.83	N
ATOM	5486	CA	GLY I		7.751	62.356	64.633	1.00 49.56	c
ATOM ATOM	5487 5488	C O	GLY I		6.734 7.074	63.435 64.613	64.915 65.004	1.00 52.99 1.00 57.80	c o
ATOM	5489	N	LYS I		5.478	63.030	65.051	1.00 57.80	N
ATOM	5490	CA	LYS I		4.399	63.962	65.352	1.00 50.83	С
MOTA	5491	С	LYS I	3 3 2 6	4.006	63.841	66.836	1.00 47.62	С
MOTA	5492	0	LYS I		3.348	62.879	67.237	1.00 55.21	ō
MOTA MOTA	5493 5494	CB CG	LYS I		3.196 3.429	63.663 63.995	64.450 62.985	1.00 60.35 1.00 72.43	c c
					3.763			, , , ,	_

MOTA	5495	CD	LYS	В	326	3.467	65.503	62.743	1.00 82.46	С
ATOM	5496	CE	LYS		326	2.087	66.119	62.908	1.00 86.36	
			LYS		326					
ATOM	5497	NZ				2.099	67.587	62.667	1.00 88.74	
MOTA	5498	N	GLN		327	4.401	64.821	67.645	1.00 36.75	
MOTA	5499	CA	GLN	В	327	4.097	64.770	69.068	1.00 33.19	С
ATOM	5500	С	GLN	В	327	2.609	64.823	69.383	1.00 31.89	С
ATOM	5501	ō	GLN			1.871	65.600	68.807	1.00 32.48	
ATOM	5502		GLN			4.822				č
		CB					65.895	69.812	1.00 26.14	
ATOM	5503	CG	GLN		327	4.941	65.663	71.317	1.00 19.26	C
ATOM	5504	CD	GLN	В	327	6.152	66.351	71.913	1.00 27.52	С
ATOM	5505	OE1	GLN	В	327	7.291	65.991	71.630	1.00 31.18	0
ATOM	5506		GLN		327	5.910	67.348	72.740	1.00 26.20	
ATOM	5507		GLY			2.180	63.992	70.323	1.00 30.12	
		N								
ATOM	5508	CA	GLY			0.779	63.952	70.699	1.00 28.50	
MOTA	5509	С	GLY			0.356	65.181	71.464	1.00 30.24	
MOTA	5510	0	GLY	В	328	1.103	66.158	71.553	1.00 32.72	0
MOTA	5511	N	TYR	В	329	-0.844	65.120	72.028	1.00 29.80	N
ATOM	5512	CA	TYR	В	329	-1.385	66.241	72.777	1.00 32.42	
ATOM	5513	c	TYR			-2.696	65.882	73.453	1.00 30.05	
ATOM	5514	0	TYR			-3.376	64.937	73.050	1.00 34.49	
MOTA	5515	CB	TYR			-1.622	67.413	71.832	1.00 43.23	C
MOTA	5516	CG	TYR	В	329	-2.507	67.045	70.657	1.00 50.66	С
ATOM	5517	CD1	TYR	В	329	-3.876	66.840	70.820	1.00 57.72	С
MOTA	5518		TYR			-1.964	66.858	69.388	1.00 49.27	C
ATOM	5519	CE1	TYR			-4.674	66.455	69.746	1.00 56.30	ř
	5520					-2.755			1.00 48.22	
MOTA			TYR				66.473	68.312		
MOTA	5521	CZ	TYR			-4.102	66.273	68.499	1.00 47.50	
ATOM	5522	ОН	TYR			-4.874	65.881	67.442	1.00 46.62	
ATOM	5523	N	GLN	В	330	-3.050	66.655	74.473	1.00 29.84	N
ATOM	5524	CA	GLN	В	330	-4.287	66.438	75.199	1.00 31.22	С
ATOM	5525	Ċ	GLN			-5.417	66.915	74.316	1.00 33.66	
ATOM	5526	õ	GLN			-5.362	67.995	73.737	1.00 31.76	
	5527									Č
ATOM		СВ	GLN			-4.286	67.234	76.497	1.00 34.22	
ATOM	5528	CG	GLN			-5.544	67.098	77.308	1.00 43.47	C
ATOM	5529	CD	GLN	В	330	-5.587	68.102	78.434	1.00 51.85	
MOTA	5530	OE1	GLN	В	330	-5.650	69.311	78.191	1.00 73.21	0
ATOM	5531		GLN			-5.543	67.616	79.679	1.00 29.07	N
ATOM	5532	N	LEU			-6.447	66.100	74.209	1.00 36.00	
	5533					-7.577	66.471	73.396	1.00 43.25	
ATOM		CA	LEU							
MOTA	5534	C	LEU			-8.654	67.027	74.308	1.00 48.53	
ATOM	5535	0	LEU	В	331	-9.072	68.176	74.162	1.00 64.23	
ATOM	5536	CB	LEU	В	331	-8.105	65.258	72.629	1.00 47.74	С
ATOM	5537	CG	LEU		331	-9.408	65.458	71.851	1.00 62.42	
ATOM	5538		LEU			-9.428	66.831	71.210	1.00 73.58	Č
	5539					-9.544	64.374	70.800	1.00 67.66	
MOTA			LEU							
ATOM	5540	N	ARG			-9.081	66.216	75.267	1.00 43.33	
MOTA	5541	CA	ARG	В	332	-10.128	66.621	76.191	1.00 51.00	
MOTA	5542	С	ARG	В	332	-9.720	66.842	77.651	1.00 54.03	
MOTA	5543	0	ARG	В	332	-8.658	66.403	78.095	1.00 58.81	
MOTA	5544	CB	ARG	В	332	-11.264	65.601	76.138	1.00 53.85	
ATOM	5545	CG	ARG		332	-12.221	65.814	74.987	1.00 65.81	. c
	5546	CD	ARG		332	-13.250	64.702	74.906	1.00 74.40	
ATOM										
MOTA	5547	NE	ARG		332	-14.437	65.091	74.142	1.00 90.15	
ATOM	5548	CZ	ARG		332	-14.417	65.591	72.908	1.00 93.10	
MOTA	5549	NH1	ARG	В	332	-13.266	65.773	72.276	1.00 90.50	
ATOM	5550	NH2	ARG	В	332	-15.554	65.910	72.300	1.00 94.95	N
MOTA	5551	N	GLN	В	333	-10.595	67.538	78.377	1.00 59.53	N
ATOM	5552	CA	GLN			-10.437	67.859	79.799	1.00 59.64	
ATOM	5553	c	GLN			-11.779	67.531	80.427	1.00 60.67	
		_		_					1 00 63 34	_
ATOM	5554	0	GLN			-12.652	66.974	79.770	1.00 63.34	
MOTA	5555	CB	GLN			-10.172	69.357	79.989	1.00 66.45	
ATOM	5556	CG	GLN			-8.737	69.784	79.800	1.00 73.50	
MOTA	5557	CD	GLN	В	333	-7.953	69.703	81.085	1.00 74.39	C
ATOM	5558	OE1	GLN	В	333	-8.156	68.792	81.885	1.00 68.78	0
MOTA	5559		GLN			-7.043	70.651	81.290	1.00 75.58	N
ATOM	5560	N	GLY			-11.942	67.873	81.697	1.00 61.52	
									1.00 64.25	
MOTA	5561	CA	GLY			-13.215	67.643	82.362		•
ATOM	5562	C	GLY			-13.545	66.316	83.026	1.00 57.75	
ATOM	5563	0	GLY			-13.184	65.241	82.540	1.00 48.01	
ATOM	5564	N	ASP			-14.252	66.418	84.151	1.00 55.93	N
ATOM	5565	CA	ASP	В	335	-14.700	65.267	84.935	1.00 56.96	C
MOTA	5566	С	ASP			-13.594	64.361	85.456	1.00 53.22	
ATOM	5567	ō	ASP			-13.828	63.188	85.763	1.00 53.10	
ATOM	5568	ČВ	ASP			-15.694	64.435	84.115	1.00 65.57	
			ASP					84.929		
ATOM	5569	CG				-16.335	63.330		1.00 74.34	<u>.</u>
MOTA	5570		ASP			-16.702	63.595	86.093	1.00 78.23	
ATOM	5571		ASP			-16.483	62.202	84.409	1.00 77.66	
ATOM	5572	N	ASN			-12.395	64.908	85.586	1.00 51.36	
ATOM	5573	CA	ASN			-11.283	64.105	86.048	1.00 45.32	
ATOM	5574	С	ASN	В	336	-11.034	63.039	85.017	1.00 37.63	
ATOM	5575	0	ASN	В	336	-11.031	61.856	85.321	1.00 34.06	6 0

ATOM	5576	CB	ASN B 3	36 -11.597	53.432	87.384	1.00 50.91	C
MOTA	5577	CG	ASN B 3		64.196	88.555	1.00 58.30	Ċ
ATOM	5578		ASN B 3		64.937	88.433	1.00 69.08	ō
ATOM	5579			36 -11.680	64.009	89.712	1.00 58.57	N
	5580	N	PHE B 3					N
MOTA					63.470	83.783	1.00 31.44	
MOTA	5581	CA		-10.581	62.562	82.700	1.00 31.17	C
ATOM	5582	C	PHE B 3		63.351	81.705	1.00 32.33	C
MOTA	5583	0	PHE B 3		64.513	81.435	1.00 36.66	0
ATOM	5584	CB	PHE B 3	37 -11.876	62.075	82.045	1.00 32.86	С
MOTA	5585	CG	PHE B 3	37 -12.306	60.699	82.488	1.00 39.46	С
MOTA	5586	CD1	PHE B 3	37 -13.653	60.415	82.718	1.00 49.81	c c
ATOM	5587		PHE B 3		59.683	82.661	1.00 47.92	Ċ
ATOM	5588			37 -14.063	59.141	83.114	1.00 54.96	Č
	5589		PHE B 3					č
MOTA					58.407	83.056	1.00 63.20	Č
ATOM	5590	CZ		37 -13.121	58.138	83.283	1.00 65.67	c
ATOM	5591	N	GLU B 3		62.737	81.189	1.00 32.09	N
ATOM	5592	CA		38 -7.849	63.373	80.189	1.00 33.18	С
ATOM	5593	С	GLU B 3		62.467	78.965	1.00 33.15	Ç
ATOM	5594	0	GLU B 3	38 -7.452	61.275	79.090	1.00 40.19	0
ATOM	5595	CB	GLU B 3	38 -6.449	63.648	80.748	1.00 25.42	С
ATOM	5596	CG	GLU B 3	38 -6.311	64.927	81.545	1.00 33.52	С
ATOM	5597	CD	GLU B 3	38 -4.855	65.332	81.751	1.00 38.56	С
ATOM	5598	OE1		38 -4.182	65.626	80.735	1.00 33.53	0
ATOM	5599	OE2			65.354	82.920	1.00 39.80	Ō
ATOM	5600	N	VAL B 3		63.028	77.781	1.00 26.69	N
ATOM	5601	CA	VAL B 3		62.236	76.571	1.00 13.92	Ċ
					62.746	75.705	1.00 13.55	č
MOTA	5602	C						
ATOM	5603	0	VAL B 3		63.847	75.155	1.00 17.78	0
ATOM	5604	CB	VAL B 3		62.257	75.715	1.00 13.19	C
ATOM	5605		VAL B 3		61.562	74.390	1.00 3.31	C
MOTA	5606	CG2		39 -10.218	61.564	76.451	1.00 3.31	C
ATOM	5607	N	TRP B 3	40 -5.611	61.937	75.590	1.00 9.29	N
ATOM	5608	CA	TRP B 3	40 -4.457	62.302	74.783	1.00 14.13	C
ATOM	5609	С	TRP B 3		61.493	73.494	1.00 17.31	C
ATOM	5610	ō		40 -5.117	60.465	73.402	1.00 26.52	0
ATOM	5611	ČВ		40 -3.166	62.065	75.574	1.00 16.12	Č
ATOM	5612	CG		40 -3.007		76.719	1.00 16.94	Č
ATOM	5613		TRP B 3		63.151	77.778	1.00 21.92	č
	5614			10 -1.962		76.902	1.00 23.88	c c
ATOM								N N
ATOM	5615	NE1			64.153	78.613	1.00 29.39	N
MOTA	5616	CE2		40 -2.245	64.671	78.096	1.00 31.49	c
ATOM	5617	CE3			64.307	76.174	1.00 28.70	c c
ATOM	5618	CZ2		40 -1.427	65.690	78.574	1.00 40.20	Ç
MOTA	5619	CZ3		40 -0.004	65.319	76.648	1.00 27.49	С
ATOM	5620	CH2	TRP B 3	40 -0.315	65.999	77.838	1.00 40.53	C
ATOM	5621	N	GLU B 3	41 -3.685	61.970	72.506	1.00 9.67	N
ATOM	5622	CA	GLU B 3	41 -3.574	61.281	71.229	1.00 7.62	С
MOTA	5623	С	GLU B 3	41 -2.411	61.810	70.387	1.00 13.01	С
ATOM	5624	ō	GLU B 3		62.994	70.425	1.00 18.84	0
MOTA	5625	ĊВ	GLU B 3		61.417	70.427	1.00 3.31	Ċ
ATOM	5626	ĊĞ		41 -4.949	62.688	69.565	1.00 25.60	č
ATOM	5627	CD	GLU B 3			68.885	1.00 30.41	č
ATOM	5628			41 -6.778		68.223	1.00 27.70	ŏ
						68.998	1.00 36.12	ŏ
MOTA	5629		GLU B 3					N
MOTA	5630	N		42 -1.803	60.918	69.620	1.00 15.38	
ATOM	5631	CA	ARG B 3		61.279	68.759	1.00 21.84	C
ATOM	5632	C		42 -0.915		67.429	1.00 17.39	C
ATOM	5633	0	ARG B 3		59.408	67.379	1.00 12.91	0
MOTA	5634	CB	ARG B 3			69.341	1.00 26.66	C
MOTA	5635	CG	ARG B 3		60.879	68.353	1.00 29.85	Ç
MOTA	5636	CD	ARG B 3	42 2.980	60.020	68.783	1.00 35.01	С
ATOM	5637	NE	ARG B 3	42 4.174	60.304	67.997	1.00 42.30	N
MOTA	5638	CZ	ARG B 3			68.209	1.00 48.51	С
ATOM	5639	NH1				69.181	1.00 43.34	N
ATOM	5640	NH2				67.461	1.00 53.48	N
ATOM	5641	N	PRO B 3		61.341	66.325	1.00 17.23	N
ATOM	5642	CA	PRO B 3			65.052	1.00 13.34	Ċ
ATOM	5643	C	PRO B 3			64.777	1.00 19.66	č
ATOM	5644	ŏ	PRO B 3			65.126	1.00 11.42	õ
	5645					64.109	1.00 14.10	č
ATOM ATOM		CB	PRO B 3			64.651	1.00 14.10	č
	5646	CG	PRO B 3					c c
ATOM	5647	CD	PRO B 3			66.130	1.00 20.84	
MOTA	5648	N	LEU B 3			64.186	1.00 29.17	N
MOTA	5649	CA	LEU B 3			63.876	1.00 39.10	c c
MOTA	5650	С	LEU B 3			62.369	1.00 48.55	С
MOTA	5651	0	LEU B 3		58.922	61.706	1.00 56.26	0
MOTA	5652	CB	LEU B 3		56.527	64.373	1.00 27.36	С
MOTA	5653	CG	LEU B 3			65.763	1.00 33.56	č
ATOM	5654		LEU B 3			66.204	1.00 40.45	С
MOTA	5655		LEU B 3			66.716	1.00 36.36	С
ATOM	5656	N	SER B 3			61.833	1.00 51.42	N

MOTA	5657	CA	SER E	3 345	2.366	56.764	60.397	1.00 50.43	С
ATOM			SER E				59.866	1.00 53.44	č
	5658	Ç			1.310	55.819			
ATOM	5659	0	SER E		0.777	55.007	60.617	1.00 59.99	0
ATOM	5660	CB	SER E	3 345	3.750	56.191	60.099	1.00 49.81	С
ATOM	5661	OG	SER E	345	4.751	56.898	60.805	1.00 65.14	0
ATOM	5662	N	GLY E		1.001	55.929	58.579	1.00 51.96	N
MOTA	5663	CA	GLY E		0.018	55.047	57.972	1.00 62.14	С
MOTA	5664	С	GLY E	3 346	-1.408	55.183	58.462	1.00 66.08	С
MOTA	5665	Ō	GLY E		-2.109	54.183	58.619	1.00 72.41	Ó
ATOM					-1.841		58.706	1.00 67.58	
	5666	N	LEU E			56.416			N
ATOM	5667	CA	LEU E		-3.206	56.680	59.158	1.00 71.85	С
MOTA	5668	С	LEU E	3 347	-3.552	56.014	60.484	1.00 70.69	С
MOTA	5669	0	LEU E	347	-4.725	55.849	60.830	1.00 75.72	0
ATOM	5670	ĊВ	LEU E		-4.205	56.224	58.090	1.00 79.33	č
MOTA	5671	CG	LEU E		-4.052	56.850	56.699	1.00 86.76	С
MOTA	5672	CD1	LEU E	347	-5.015	56.184	55.726	1.00 94.59	С
MOTA	5673	CD2	LEU E	3 347	-4.311	58.350	56.771	1.00 93.49	С
ATOM	5674	N	ALA E	348	-2.522	55.622	61.221	1.00 64.54	N
ATOM	5675	CA	ALA E		-2.712	54.974	62.508	1.00 55.40	Ċ
		_							č
MOTA	5676	C	ALA E		-2.570	56.034	63.588	1.00 47.16	Ç
ATOM	5677	0	ALA E		-1.744	56.943	63.472	1.00 52.56	0
MOTA	5678	CB	ALA E	348	-1.680	53.882	62.696	1.00 65.49	С
ATOM	5679	N	TRP E	349	-3.378	55.921	64.635	1.00 33.00	N
ATOM	5680	CA	TRP E		-3.341	56.885	65.724	1.00 29.96	Ċ
MOTA	5681	C		3 3 4 9	-3.239	56.227	67.086	1.00 24.51	C
MOTA	5682	0		349	-3.819	55.166	67.329	1.00 28.15	0
MOTA	5683	CB	TRP E	349	-4.583	57.764	65.694	1.00 30.99	C
MOTA	5684	CG	TRP E		-4.627	58.696	64.547	1.00 39.58	Ċ
MOTA	5685		TRP E		-4.546	58.379	63.209	1.00 48.37	č
									Č
MOTA	5686		TRP E		-4.829	60.101	64.614	1.00 39.41	С
ATOM	5687	NE1	TRP E	349	-4.691	59.510	62.447	1.00 44.17	N
MOTA	5688	CE2	TRP E	3 3 4 9	-4.869	60.583	63.285	1.00 44.56	С
MOTA	5689	CE3	TRP E	349	-4.983	61.005	65.664	1.00 48.26	С
MOTA	5690		TRP E		-5.065	61.938	62.988	1.00 51.67	Č
MOTA	5691	CZ3			-5.174	62.342	65.372	1.00 53.35	Ç
MOTA	5692	CH2	TRP E		-5.214	62.799	64.048	1.00 55.52	С
ATOM	5693	N	ALA E	3 3 5 0	-2.496	56.874	67.976	1.00 21.97	N
MOTA	5694	CA	ALA E	350	-2.317	56.361	69.318	1.00 15.04	С
MOTA	5695	Ċ	ALA E		-3.203	57.220	70.204	1.00 13.29	č
MOTA	5696	0_	ALA E		-3.326	58.427	69.956	1.00 21.97	0
ATOM	5697	CB	ALA E	350	-0.859	56.477	69.724	1.00 14.88	С
ATOM	5698	N	VAL E	351	-3.828	56.615	71.216	1.00 11.43	N
ATOM	5699	CA	VAL E		-4.700	57.377	72.109	1.00 16.42	С
	5700		VAL E			57.023	73.587	1.00 14.52	č
ATOM		Č			-4.553				
ATOM	5701	0	VAL E		-4.475	55.848	73.942	1.00 20.61	0
ATOM	5702	СВ	VAL E	351	-6.187	57.209	71.731	1.00 14.15	С
ATOM	5703	CG1	VAL E	351	-7.039	58.140	72.591	1.00 18.62	С
ATOM	5704		VAL E		-6.402	57.518	70.257	1.00 10.92	С
ATOM	5705		ALA E			58.045	74.442	1.00 7.24	N
		N			-4.543				
MOTA	5706	CA	ALA E		-4.405	57.836	75.878	1.00 12.07	Ç
MOTA	5707	С	ALA E	3 352	-5.681	58.164	76.640	1.00 5.81	С
ATOM	5708	0	ALA E	352	-6.467	59.021	76.239	1.00 3.31	0
ATOM	5709	CB	ALA E	352	-3.249	58.667	76.423	1.00 31.41	С
ATOM	5710	N	MET E		-5.871	57.467	77.750	1.00 9.84	N
MOTA	5711	CA	MET E		-7.042	57.658	78.589	1.00 22.44	Č
MOTA	5712	С	MET E		-6.618	57.603	80.066	1.00 27.10	С
MOTA	5713	0	MET E	353	-6.460	56.525	80.650	1.00 32.99	0
ATOM	5714	CB	MET E		-8.077	56.572	78.267	1.00 19.22	С
ATOM	5715	CG	MET E		-9.415	57.108	77.759	1.00 18.91	č
							76 070		
ATOM	5/16	SD	MET E		-9.999	56.263	76.279	1.00 26.72	S
ATOM	5717	CE	MET E		-10.279	54.594	76.866	1.00 38.91	c
ATOM	5718	N	ILE E		-6.439	58.783	80.654	1.00 21.63	N
ATOM	5719	CA	ILE E		-6.008	58.920	82.037	1.00 19.84	С
ATOM	5720	C	ILE E		-7.171	59.205	82.975	1.00 20.11	С
ATOM	5721	ŏ	ILE B		-7.959	60.121	82.716	1.00 23.90	õ
ATOM	5722					60.090	82.193	1.00 23.50	č
		CB	ILE B		-5.036				Č
ATOM	5723		ILE E		-4.079	60.144	81.012	1.00 20.37	C
MOTA	5724		ILE B		-4.258	59.929	83.481	1.00 26.13	С
MOTA	5725	CD1	ILE B	354	-3.386	61.474	80.867	1.00 37.14	С
ATOM	5726	N	ASN E		-7.276	58.431	84.056	1.00 23.98	N
ATOM	5727	CA	ASN E		-8.324	58.649	85.041	1.00 28.05	Ċ
									č
MOTA	5728	Ç	ASN B		-7.701	59.455	86.179	1.00 25.20	c
MOTA	5729	0	ASN E		-7.084	58.905	87.080	1.00 25.36	0
ATOM	5730	CB	ASN E	355	-8.877	57.308	85.545	1.00 22.56	c c
MOTA	5731	CG	ASN E		-9.823	57.466	86.735	1.00 21.05	c
ATOM	5732		ASN E		-10.566	58.445	86.849	1.00 32.29	ŏ
						56.487			
ATOM	5733		ASN E		-9.803		87.620	1.00 17.99	N
MOTA	5734	N	ARG E		-7.841	60.770	86.115	1.00 20.51	N
ATOM	5735	CA	ARG E	356	-7.279	61.627	87.132	1.00 31.23	С
MOTA	5736	С	ARG E		-8.053	61.623	88.446	1.00 35.46	С
ATOM	5737	ō	ARG E		-7.897	62.550	89.260	1.00 46.20	ŏ
	• •	-						3.00 10.20	Ū

							06 610		_
ATOM	5738	СВ	ARG B		-7.169	63.055	86.612	1.00 38.86	C
ATOM	5739	CG	ARG E		-6.047	63.244	85.616	1.00 43.53	C
ATOM	5740	CD	ARG B		-4.692	62.814	86.195	1.00 50.19	С
ATOM	5741	NE	ARG B	356	-4.092	63.775	87.134	1.00 59.43	N
ATOM	5742	CZ	ARG B	356	-3.703	65.010	86.815	1.00 63.12	С
ATOM	5743	NH1	ARG B	356	-3.850	65.459	85.575	1.00 65.44	N
ATOM	5744		ARG B		-3.147	65.793	87.730	1.00 62.05	N
ATOM	5745	N	GLN B		~8.870	60.592	88.673	1.00 28.87	N.
ATOM	5746	CA	GLN B		-9.633	60.512	89.928	1.00 33.47	C
ATOM	5747	C	GLN B		-8.962	59.676	91.039	1.00 30.43	c
ATOM	5748	0	GLN B		-9.178	58.469	91.159	1.00 36.76	0
ATOM	5749	CB	GLN B		-11.035	59.986	89.645	1.00 40.97	С
ATOM	5750	CG	GLN B		-11.891	59.925	90.876	1.00 54.27	č
ATOM	5751	CD	GLN B	357	-13.338	60.217	90.596	1.00 62.67	С
ATOM	5752	OE1	GLN B	357	-13.673·	61.300	90.143	1.00 69.07	0
ATOM	5753	NE2	GLN B	357	-14.205	59.251	90.854	1.00 65.72	N
ATOM	5754	N	GLU B	358	-8.155	60.350	91.849	1.00 26.80	
ATOM	5755	CA	GLU B	358	-7.399	59.741	92.948	1.00 32.29	C
ATOM	5756	C	GLU B		-8.125	58.769	93.898	1.00 28.60	
ATOM	5757	ō	GLU B		-7.482	57.963	94.573	1.00 30.41	ŏ
ATOM	5758	ČВ	GLU B		-6.779	60.857	93.797	1.00 43.79	č
									c
ATOM	5759	CG	GLU B		-5.919	61.873	93.036	1.00 48.64	Č
ATOM	5760	CD	GLU B		-4.510	61.379	92.749	1.00 44.93	C
ATOM	5761		GLU B		-3.894	60.773	93.649	1.00 42.30	0
ATOM	5762		GLU B		-4.012	61.616	91.629	1.00 40.88	0
MOTA	5763	N	ILE B		-9.448	58.848	93.968	1.00 27.88	
ATOM	5764	CA	ILE B		-10.202	57.989	94.875	1.00 34.30	С
ATOM	5765	С	ILE B	359	-11.295	57.155	94.204	1.00 34.85	С
ATOM	5766	0	ILE B	359	-11.694	57.430	93.082	1.00 37.79	0
ATOM	5767	СВ	ILE B		-10.827	58.840	96.002	1.00 39.33	Ċ
ATOM	5768		ILE B		-11.420	57.935	97.086	1.00 31.29	Ċ
ATOM	5769		ILE B		-11.877	59.774	95.420	1.00 43.50	č
ATOM	5770		ILE B		-11.978	58.692	98.238	1.00 40.02	C
ATOM	5771								
		N	GLY B		-11.764	56.123	94.897	1.00 39.25	N
ATOM	5772	CA	GLY B		-12.804	55.260	94.359	1.00 44.05	C
ATOM	5773	Ç	GLY B		-12.265	54.016	93.671	1.00 42.72	C
ATOM	5774	0	GLY B		-11.394	53.316	94.196	1.00 39.94	0
ATOM	5775	N	GLY B		-12.795	53.733	92.488	1.00 46.69	N
ATOM	5776	CA	GLY B	361	-12.347	52.574	91.742	1.00 49.53	С
ATOM	5 <i>777</i>	С	GLY B	361	-12.208	52.907	90.269	1.00 52.50	C
MOTA	5778	0	GLY B	361	-12.057	54.085	89.923	1.00 62.49	0
ATOM	5779	N	PRO B	362	-12.257	51.898	89.378	1.00 48.87	N
ATOM	5780	CA	PRO B	362	-12.136	52.099	87.938	1.00 44.58	С
ATOM	5781	C	PRO B		-13.434	52.656	87.376	1.00 42.25	С
ATOM	5782	ō	PRO B		-14.472	52.010	87.469	1.00 43.66	Ō
ATOM	5783	ČВ	PRO B		-11.847	50.693	87.425	1.00 43.79	
ATOM	5784	ĊĞ	PRO B		-12.723	49.871	88.278	1.00 41.53	č
ATOM	5785	CD	PRO B		-12.502	50.474	89.669	1.00 48.21	č
ATOM	5786		ARG B		-13.371		86.803	1.00 41.38	
		N			-14.551	53.854	86.236	1.00 46.33	C
ATOM	5787	CA	ARG B			54.477			
ATOM	5788	C	ARG B		-14.622	54.077	84.783	1.00 45.49	
MOTA	5789	0	ARG B		-13.739	53.375	84.299	1.00 51.49	0
ATOM	5790	СВ	ARG B		-14.458	55.991	86.422	1.00 54.78	
ATOM	5791	CG	ARG B		-14.145	56.315	87.872	1.00 63.13	C
ATOM	5792	CD	ARG B	363	-14.508	57.715	88.292	1.00 53.78	
ATOM	5793	NE	ARG B		-13.570	58.711	87.803	1.00 41.54	N
ATOM	5794	CZ	ARG B	363	-13.743	59.405	86.689	1.00 31.79	C
ATOM	5795	NH1	ARG B	363	-14.818	59.209	85.943	1.00 17.21	N
ATOM	5796	NH2	ARG B	363	-12.856	60.317	86.336	1.00 43.49	N
ATOM	5797	N	SER B		-15.669	54.479	84.079	1.00 44.85	N
ATOM	5798	CA	SER B		-15.755	54.114	82.672	1.00 49.86	С
ATOM	5799	c	SER B		-15.912	55.371	81.838	1.00 53.15	č
ATOM	5800	ò	SER B		-16.669	56.272	82.203	1.00 62.86	ŏ
ATOM	5801	СВ	SER B		-16.929	53.162	82.428	1.00 45.42	č
MOTA	5802	OG					82.803		Ö
			SER B		-18.156	53.755	80.740	1.00 51.36 1.00 54.75	Ŋ
ATOM	5803	N	TYR B		-15.166	55.441			
ATOM	5804	CA	TYR B		-15.238	56.584	79.850	1.00 55.94	C
ATOM	5805	C	TYR B		-15.648	56.093	78.457	1.00 56.83	C
ATOM	5806	0	TYR B		-15.192	55.038	77.988	1.00 58.68	0
ATOM	5807	CB	TYR B		-13.893	57.319	79.786	1.00 55.40	C
MOTA	5808	CG	TYR B		-14.018	58.685	79.157	1.00 60.79	c c
ATOM	5809		TYR B		-14.730	59.699	79.795	1.00 65.68	С
MOTA	5810	CD2	TYR B	365	-13.479	58.950	77.892	1.00 56.75	Ċ
ATOM	5811		TYR B		-14.911	60.947	79.190	1.00 65.13	С
ATOM	5812		TYR B		-13.651	60.194	77.279	1.00 58.15	С
ATOM	5813	CZ	TYR B		-14.370	61.190	77.933	1.00 63.09	С
ATOM	5814	ОН	TYR B		-14.553	62.424	77.337	1.00 65.91	ŏ
MOTA	5815	N	THR B		-16.511	56.871	77.807	1.00 55.80	N
ATOM	5816	CA	THR B		-17.028	56.539	76.490	1.00 52.06	c .:
MOTA	5817	c	THR B		-16.975	57.753	75.584	1.00 49.80	
ATOM	5818	ò	THR B		-17.385	58.838	75.986	1.00 52.16	
011	5010	Ü	**** D		-11.303	JU. 0 JU		2.00 32.10	U

МОТА	5819	СВ	тμр	R	366	-18.489	56.112	76.597	1 00	53.56	С
ATOM	5820		THR			-19.228	57.135	77.280		58.14	ŏ
ATOM	5821		THR			-18.611	54.836	77.381		53.03	č
ATOM	5822	N			367	-16.475	57.581	74.364		46.90	N
	5823	CA			367	-16.403	58.695	73.406		53.96	Č
ATOM	5824	c			367	-16.819	58.320	71.997		52.93	č
MOTA											
ATOM	5825	0			367	-16.926	57.139	71.659		53.28	0
MOTA	5826	CB			367	-14.985	59.305	73.272		58.74	C
ATOM	5827		ILE			-13.924	58.202	73.250		58.91	c c c
MOTA	5828		ILE			-14.767	60.342	74.351		63.43	Ċ
MOTA	5829		ILE			-13.997	57.279	72.051		50.07	C
ATOM	5830	N			368	-17.027	59.345	71.173		59.91	N
ATOM	5831	CA			368	-17.417	59.149	69.781		62.43	c
MOTA	5832	c			368	-16.222	58.775	68.898		57.88	C
ATOM	5833	0			368	-15.451	59.640	68.465		57.96	0
MOTA	5834	CB			368	-18.088	60.410	69.245		73.79	c
MOTA	5835	N			369	-16.074	57.477	68.662		51.51	N
MOTA	5836	CA			369	-15.015	56.957	67.826		49.72	C
MOTA	5837	C			369	-14.660	57.962	66.746	-	50.98	c
MOTA	5838	0			369	-13.489	58.237	66.484		50.73	ō
MOTA	5839	CB			369	-15.474	55.652	67.166		54.09	c c
MOTA	5840		VAL			-14.505	55.219	66.093		56.99	c
MOTA	5841		VAL			-15.619	54.588	68.218		61.48	N N
MOTA	5842	N			370	-15.692	58.513	66.124		54.79	C
ATOM	5843	CA			370	-15.525	59.492	65.057		59.90	Ċ
ATOM	5844	C			370	-14.701	60.706	65.479		55.69	ò
ATOM	5845	O CB			370 370	-13.558	60.871 59.944	65.058 64.563		59.19 69.60	c
MOTA MOTA	5846 5847	CB N			371	-16.897 -15.289	61.548	66.318		48.90	N
MOTA					371	-14.619	62.747	66.783		48.25	Č
MOTA MOTA	5848 5849	CA C			371	-13.358	62.423	67.593		44.02	c
ATOM	5850	ò			371	-13.095	63.035	68.629		46.23	Ö
ATOM	5851	СВ			371	-15.584	63.599	67.623		56.08	č
ATOM	5852	OG			371	-15.871	62.996	68.880		58.94	ŏ
MOTA	5853	N			372	-12.582	61.456	67.116		40.16	N
ATOM	5854	CA			372	-11.341	61.088	67.780		38.78	č
ATOM	5855	c			372.	-10.120	61.503	66.958		41.62	č
ATOM	5856	ō			372	-9.564	62.587	67.158		47.58	ŏ
ATOM	5857	СB			372	-11.301	59.578	68.039		37.09	č
ATOM	5858	CG			372	-10.124	59.082	68.900		30.31	č
ATOM	5859		LEU			-10.025	59.910	70.177		31.09	č
ATOM	5860		LEU			-10.307	57.613	69.249		19.07	č
ATOM	5861	N			373	-9.709	60.637	66.035		40.17	N
ATOM	5862	CA			373	-8.552	60.924	65.202		46.24	c
ATOM	5863	c			373	-8.841	62.101	64.298		49.50	č
ATOM	5864	ŏ			373	-8.789	61.984	63.081		40.52	ō
ATOM	5865	N			374	-9.135	63.243	64.909		58.63	N
ATOM	5866	CA			374	-9.455	64.466	64.191		64.48	Ċ
ATOM	5867	C			374	-10.535	64.197	63.172		66.08	C
ATOM	5868	ŏ			374	-10.728	64.986	62.253		68.10	0
ATOM	5869	ČВ			374	-8.209	65.027	63.496		64.15	c c
ATOM	5870	CG			374	-7.864	66.432	63.942		72.20	С
MOTA	5871	CD			374	-6.431	66.800	63.593	1.00	72.70	Ċ
MOTA	5872	CE			374	-6.034	68.156	64.184		77.53	C
MOTA	5873	NZ			374	-6.075	68.198	65.684	1.00	72.68	N
ATOM	5874	N	GLY	В	375	-11.233	63.078	63.349	1.00	66.41	N
MOTA	5875	CA	GLY	В	375	-12.292	62.693	62.434	1.00	62.04	С
MOTA	5876	С	GLY	В	375	-11.839	61.672	61.405	1.00	60.69	С
MOTA	5877	0	GLY	В	375	-12.635	60.857	60.940	1.00	61.43	0
MOTA	5878	N	VAL	В	376	-10.555	61.718	61.058	1.00	58.18	N
MOTA	5879	CA			376	-9.959	60.815	60.078		57.67	С
MOTA	5880	С	VAL	В	376	-9.950	59.361	60.521	1.00	61.90	С
ATOM	5881	0	VAL	В	376	-10.806	58.585	60.107		71.76	0
ATOM	5882	CB			376	-8.509	61.216	59.756		51.56	С
MOTA	5883		VAL			-7.872	60.178	58.856		54.68	Č
ATOM	5884		VAL			-8.488	62.566	59.082		63.57	c
MOTA	5885	N			377	-8.971	58.989	61.344		57.39	N
MOTA	5886	CA			377	-8.873	57.621	61.828		54.98	c
ATOM	5887	C			377	-10.246	57.209	62.316		57.77	c
MOTA	5888	0			377	-10.799	57.825	63.224		58.49	0
MOTA	5889	СВ			377	-7.871	57.541	62.944		46.92	C
ATOM	5890	N			378	-10.781	56.166	61.690		59.13	N
ATOM	5891	CA			378	-12.109	55.624	61.982		63.50	C
MOTA	5892	C			378	-13.079	55.952	60.868		66.64	Č
MOTA	5893	0			378	-14.303	55.884	61.041 63.290		72.37	0
ATOM	5894	CB			378	-12.660	56.162	64.708			s
ATOM ATOM	5895 5896	SG			378	-11.718	55.523	59.716		88.55	S N
ATOM ATOM	5896 5897	N CA			379 379	-12.519 -13.304	56.313 56.641	58.523		66.49 65.90	C
MOTA	5898	C			379	-13.304	55.783	57.384		64.13	Č
ATOM	5899	ō			379	-11.690	56.061	56.844		61.36	ŏ
		-		_		21.070					•

ATOM	5900	СВ	ASN B	379	-13.142	58.118	58.184	1.00 70.43	С
ATOM	5901	CG	ASN B	379	-14.141	58.591	57.153	1.00 77.67	č
MOTA	5902		ASN B		-15.339	58.673	57.422	1.00 83.76	0
MOTA	5903		ASN B		-13.657	58.888	55.956	1.00 79.95	N
ATOM	5904	N	PRO B		-13.471	54.711	57.023	1.00 67.27	N
MOTA MOTA	5905 5906	CA C	PRO B		-14.742 -14.578	54.268	57.607	1.00 73.01	C
ATOM	5907	ò	PRO B		-15.208	53.382 53.604	58.854 59.891	1.00 75.60	0
ATOM	5908	СВ	PRO B		-15.391	53.513	56.451	1.00 81.41	č
ATOM	5909	CG	PRO B		-14.213	52.835	55.823	1.00 75.92	č
MOTA	5910	CD	PRO B		-13.122	53.883	55.858	1.00 67.18	Č
MOTA	5911	N	ALA B		-13.693	52.394	58.742	1.00 72.14	N
ATOM	5912	CA	ALA B		-13.406	51.442	59.818	1.00 70.13	c c
ATOM	5913	C	ALA B	2.2	-12.163	51.751	60.659	1.00 68.84	C
ATOM ATOM	5914 5915	0	ALA B ALA B		-11.176 -13.287	52.278 50.038	60.163	1.00 60.19	0 C
ATOM	5916	N	CYS B		-12.227	51.388	59.228 61.936	1.00 75.02 1.00 71.46	N
ATOM	5917	CA	CYS B		-11.132	51.594	62.870	1.00 71.39	č
ATOM	5918	C	CYS B		-10.856	50.319	63.596	1.00 68.84	č
ATOM	5919	0	CYS B	382	-11.741	49.779	64.254	1.00 72.06	. 0
ATOM	5920	СВ	CYS B		-11.486	52.640	63.920	1.00 75.13	С
ATOM	5921	SG	CYS B		-10.471	54.142	63.895	1.00 80.32	S
ATOM	5922 5923	N CA	PHE B		-9.634 -9.328	49.830	63.498 64.232	1.00 63.36	N C
ATOM ATOM	5924	C	PHE B		-8.533	48.624 49.057	65.453	1.00 61.05 1.00 54.93	Č
ATOM	5925	õ	PHE B		-7.405	49.531	65.330	1.00 55.67	ŏ
ATOM	5926	СВ	PHE B		-8.534	47.636	63.387	1.00 70.41	С
ATOM	5927	CG	PHE B		-8.450	46.264	64.004	1.00 83.99	С
ATOM	5928		PHE B		-9.587	45.650	64.527	1.00 87.52	c c c
MOTA	5929		PHE B		-7.248	45.574	64.036	1.00 96.23	C
MOTA MOTA	5930 5931		PHE B		-9.520 -7.168	44.380 44.299	65.088 64.595	1.00 98.04	Ċ
MOTA	5932	CZ	PHE B		-8.311	43.700	65.113	1.00103.10	č
ATOM	5933	N	ILE B		-9.141	48.900	66.624	1.00 48.57	Й
ATOM	5934	CA	ILE B		-8.516	49.297	67.867	1.00 45.07	C
ATOM	5935	C	ILE B		-8.029	48.124	68.677	1.00 48.37	С
ATOM	5936	0	ILE B		-8.790	47.219	69.009	1.00 51.85	0
ATOM	5937	CB	ILE B		-9.494	50.062	68.742	1.00 48.28	C
MOTA MOTA	5938 5939		ILE B		-10.259 -8.747	51.056 50.769	67.887 69.862	1.00 48.39 1.00 55.97	c c
MOTA	5940		ILE B		-11.433	51.663	68.581	1.00 53.13	· č
ATOM	5941	N	THR B		-6.757	48.152	69.019	1.00 49.48	й
MOTA	5942	CA	THR B		-6.202	47.085	69.807	1.00 48.02	С
ATOM	5943	С	THR B		-5.663	47.726	71.080	1.00 42.47	С
ATOM	5944	0	THR B		-4.704	48.508	71.034	1.00 46.44	0
MOTA MOTA	5945 5946	CB	THR B		-5.064	46.374	69.025	1.00 51.77	C
MOTA	5947		THR B		-3.884 -5.478	47.189 46.134	69.016 67.568	1.00 60.29 1.00 51.29	č
ATOM	5948	N	GLN B		-6.299	47.436	72.214	1.00 33.49	N
ATOM	5949	CA	GLN B		-5.819	48.012	73.468	1.00 27.25	С
MOTA	5950	С	GLN B		-4.364	47.633	73.517	1.00 30.82	С
ATOM	5951	0	GLN B		-4.022	46.471	73.370	1.00 43.33	0
MOTA MOTA	5952 5953	CB	GLN B GLN B		-6.537	47.442 48.141	74.691 75.964	1.00 19.21 1.00 29.27	c c
ATOM	5954	CG CD	GLN B		-6.116 -6.988	47.796	77.157	1.00 23.27	č
ATOM	5955		GLN B		-6.554	47.102	78.062	1.00 39.89	ŏ
ATOM	5956		GLN B		-8.224	48.281	77.158	1.00 34.21	N
ATOM	5957	N	LEU B		-3.495	48.615	73.677	1.00 27.39	N
MOTA	5958	CA	LEU B		-2.080	48.313	73.699	1.00 18.51	C
ATOM	5959	C	LEU B		-1.580	48.409	75.117	1.00 22.23	C
ATOM ATOM	5960 5961	O CB	LEU B LEU B		-0.413 -1.329	48.123 49.294	75.387 72.796	1.00 28.65 1.00 14.64	0 C
ATOM	5962	CG	LEU B		-0.052	48.767	72.147	1.00 20.38	č
MOTA	5963		LEU B		-0.378	47.537	71.320	1.00 23.24	С
MOTA	5964		LEU B		0.559	49.836	71.259	1.00 31.00	¢
ATOM	5965	N	LEU B		-2.483	48.802	76.019	1.00 21.17	N
ATOM	5966	CA	LEU B		-2.172	48.986	77.446	1.00 19.64	C
ATOM ATOM	5967 5968	C O	LEU B		-3.451	49.247 49.874	78.251 77.769	1.00 19.25 1.00 21.14	C 0
MOTA	5969	СВ	LEU B		-4.398 -1.208	50.163	77.625	1.00 21.14	c
ATOM	5970	CG	LEU B		0.184	49.979	78.220	1.00 17.52	č
MOTA	5971	CD1	LEU B	388	0.726	48.600	77.929	1.00 12.74	c c
ATOM	5972		LEU B		1.098	51.056	77.638	1.00 21.55	C
ATOM	5973	N	PRO B		-3.468	48.827	79.516 80.203	1.00 20.41	N C
MOTA MOTA	5974 5975	CA C	PRO B		-2.386 -2.324	48.117 46.606	79.934	1.00 33.25	c
MOTA	5976	ŏ	PRO B		-1.639	45.883	80.649	1.00 41.33	ŏ
MOTA	5977	ČВ	PRO B		-2.695	48.413	81.657	1.00 35.42	č
MOTA	5978	CG	PRO B	389	-4.191	48.283	81.687	1.00 28.80	C C
MOTA	5979	CD	PRO B		-4.622	49.026	80.413	1.00 19.85	
MOTA	5980	N	VAL B	240	-3.007	46.124	78.897	1.00 45.28	N

ATOM	5981	CA	VAL B	390	-3.011	44.686	78.647	1.00 50.03	С
					-3.034	44.223	77.197		
ATOM	5982	Č	VAL B					1.00 56.62	C
ATOM	5983	0	VAL B		-3.369	43.075	76.904	1.00 61.87	0
ATOM	5984	CB	VAL B		-4.186	44.036	79.370	1.00 48.80	С
ATOM	5985		VAL B		-4.098	44.301	80.849	1.00 42.23	С
ATOM	5986	CG2	VAL B	390	-5.479	44.604	78.813	1.00 53.36	С
MOTA	5987	N	LYS B	391	-2.657	45.098	76.283	1.00 59.77	N
ATOM	5988	CA	LYS B	391	-2.647	44.723	74.870	1.00 60.79	С
ATOM	5989	Ċ	LYS B		-3.673	43.649	74.510	1.00 56.27	č
ATOM	5990	ŏ	LYS B		-3.330	42.473	74.361	1.00 51.28	ŏ
ATOM	5991	CB	LYS B		-1.251	44.248	74.446	1.00 60.41	c
ATOM	5992	CG	LYS B		-1.102	44.083	72.920	1.00 65.59	C
ATOM	5993	CD	LYS B		0.300	43.695	72.407	1.00 67.80	C
ATOM	5994	CE	LYS B	391	0.479	43.992	70.897	1.00 68.90	С
MOTA	5995	NZ	LYS B	391	0.432	42.704	70.094	1.00 67.32	N
ATOM	5996	N	ARG B	392	-4.931	44.070	74.395	1.00 55.13	N
ATOM	5997	CA	ARG B		-6.023	43.182	74.036	1.00 55.86	C
ATOM	5998	Ċ	ARG B		-6.479	43.580	72.628	1.00 54.10	č
	5999		ARG B		-6.277	44.716	72.191	1.00 54.13	ŏ
ATOM		0							
ATOM	6000	СВ	ARG B		-7.180	43.342	75.023	1.00 64.65	c
ATOM	6001	CG	ARG B		-8.006	42.078	75.224	1.00 78.88	Č
ATOM	6002	CD	ARG B		-9.451	42.397	75.614	1.00 87.47	С
ATOM	6003	NE	ARG B	392	-9.546	43.414	76.664	1.00 98.24	N
ATOM	6004	CZ	ARG B	392	-9.077	43.272	77.903	1.00102.06	С
ATOM	6005	NH1	ARG B		-8.475	42.148	78.263	1.00104.13	N
ATOM	6006		ARG B		-9.201	44.260	78.784	1.00102.28	N
ATOM	6007	N	LYS B		-7.122	42.651	71.933	1.00 56.38	N
	-				-7.587	42.894	70.574		Ċ
ATOM	6008	CA	LYS B					1.00 57.73	
ATOM	6009	C	LYS B		-9.068	43.246	70.506	1.00 62.23	C
ATOM	6010	0	LYS B		-9.912	42.361	70.385	1.00 70.67	0
ATOM	6011	СВ	LYS B	393	-7.336	41.656	69.717	1.00 60.70	С
ATOM	6012	CG	LYS B	393	-6.324	41.828	68.591	1.00 64.98	С
MOTA	6013	CD	LYS B	393	-6.131	40.503	67.865	1.00 69.41	c
ATOM	6014	CE	LYS B		-4.949	40.549	66.911	1.00 66.84	С
ATOM	6015	NZ	LYS B		-4.704	39.218	66.285	1.00 71.48	N
ATOM	6016	N	LEU B		-9.392	44.531	70.581	1.00 59.79	N
			LEU B		-10.791	44.944	70.499	1.00 57.57	Ċ
ATOM	6017	CA							Č
MOTA	6018	C	LEU B		-11.208	44.787	69.049	1.00 60.43	c
MOTA	6019	0	LEU B		-10.345	44.726	68.174	1.00 65.60	0
ATOM	6020	CB	LEU B	394	-10.917	46.388	70.946	1.00 54.96	Ċ
ATOM	6021	CG	LEU B	394	-10.267	46.558	72.318	1.00 52.67	С
MOTA	6022	CD1	LEU B	394	-10.265	48.016	72.704	1.00 60.31	С
ATOM	6023	CD2	LEU B	394	-11.018	45.729	73.341	1.00 64.58	c
ATOM	6024	N	GLY B		-12.511	44.729	68.784	1.00 64.48	N
MOTA	6025	CA	GLY B		-12.971	44.551	67.409	1.00 72.78	Ċ
ATOM	6026	c	GLY B		-12.821	45.719	66.438	1.00 71.45	č
								1.00 75.01	ŏ
ATOM	6027	0	GLY B		-12.020	46.629	66.660		
ATOM	6028	N	PHE B		-13.578	45.677	65.340	1.00 67.34	N
MOTA	6029	CA	PHE B		-13.554	46.742	64.331	1.00 64.20	C
MOTA	6030	С	PHE B		-14.505	47.844	64.784	1.00 55.21	Ç
ATOM	6031	0	PHE B	396	-15.501	47.572	65.441	1.00 57.53	0
MOTA	6032	CB	PHE B	396	-14.028	46.216	62.968	1.00 82.65	С
MOTA	6033	CG	PHE B	396	-13.033	45.316	62.265	1.00102.32	С
ATOM	6034		PHE B		-12.184	45.818	61.281	1.00111.78	С
ATOM	6035		PHE B		-12.960	43.961	62.570	1.00109.39	c
	6036		PHE B		-11.276	44.985	60.615	1.00115.13	č
ATOM								1.00113.13	č
ATOM	6037		PHE B		-12.055	43.121	61.910		Č
ATOM	6038	CZ	PHE B		-11.216	43.635	60.930	1.00113.32	
ATOM	6039	N	TYR B		-14.201	49.085	64.434		N
MOTA	6040	CA	TYR B		-15.059	50.198	64.807	1.00 57.23	C
ATOM	6041	Ç	TYR B		-15.357	51.085	63.607	1.00 61.72	C
ATOM	6042	0	TYR B		-14.452	51.486	62.879	1.00 60.46	. 0
ATOM	6043	CB	TYR B	397	-14.412	51.024	65.919	1.00 64.37	C
ATOM	6044	CG	TYR B	397	-14.472	50.359	67.274	1.00 77.41	C
ATOM	6045		TYR B		-13.654	49.276	67.584	1.00 86.02	С
MOTA	6046		TYR B		-15.385	50.790	68.236	1.00 87.56	С
ATOM	6047		TYR B		-13.746	48.633	68.823	1.00 95.71	
ATOM	6048		TYR B		-15.490	50.158	69.478	1.00 92.49	ř
			TYR B				69.766	1.00 96.36	c c
MOTA	6049	CZ			-14.669	49.078		1.00 92.61	ō
ATOM	6050	ОН	TYR B		-14.784	48.436	70.984		
ATOM	6051	N	GLU B		-16.631	51.373	63.375	1.00 67.89	N
MOTA	6052	CA	GLU B		-16.990	52.224	62.253	1.00 76.13	c
MOTA	6053	С	GLU B		-16.839	53.649	62.682	1.00 74.01	C
MOTA	6054	0	GLU B		-16.544	53.937	63.844	1.00 75.69	0
ATOM	6055	CB	GLU B	398	-18.430	51.980	61.808	1.00 86.18	С
ATOM	6056	CG	GLU B		-18.589	50.683	61.075	1.00107.33	С
MOTA	6057	CD	GLU B		-17.867	49.567	61.790	1.00123.23	c c
ATOM	6058		GLU B		-18.252	49.262	62.939	1.00129.75	Ō
ATOM	6059		GLU B		-16.904	49.013	61.217	1.00128.47	ŏ
ATOM	6060	N	TRP B		-17.030	54.547	61.732	1.00 70.53	N
ATOM						55.953	62.032	1.00 69.74	C
A I ON	6061	CA	TRP B	377	-16.924	درد.رر	02.032	2.00 03.74	C

ATOM	6062	С	TRP E	3 399	-17.957	56.198	63.122	1.00 69.71	С
	6063	ŏ	TRP E		-17.608	56.597	64.233	1.00 70.76	ŏ
ATOM									
MOTA	6064	CB	TRP E		-17.228	56.778	60.783	1.00 68.11	Ç
MOTA	6065	CG	TRP E	3 399	-16.673	58.158	60.844	1.00 69.78	С
MOTA	6066	CD1	TRP E	3 399	-15.362	58.525	60.738	1.00 68.46	С
MOTA	6067		TRP E		-17.410	59.361	61.072	1.00 76.78	č
MOTA	6068		TRP E		-15.235	59.884	60.888	1.00 71.48	N
MOTA	6069	CE2	TRP E	3 399	-16.479	60.423	61.095	1.00 78.32	С
MOTA	6070	CE3	TRP E	3 399	-18.772	59.647	61.264	1.00 85.58	С
MOTA	6071		TRP F		-16.867	61.755	61.304	1.00 86.28	Ċ
			TRP E		-19.160	60.974	61.473	1.00 89.12	č
ATOM	6072	CZ3							
MOTA	6073	CH2	TRP E		-18.209	62.009	61.491	1.00 91.47	С
ATOM	6074	N	THR E	3 400	-19.222	55.911	62.816	1.00 68.79	N
ATOM	6075	CA	THR E	3 400	-20.306	56.105	63.784	1.00 74.00	С
ATOM	6076	c	THR E		-19.941	55.562	65.162	1.00 77.61	Ċ
								1.00 85.51	
MOTA	6077	0	THR E		-20.103	56.252	66.173		0
MOTA	6078	CB	THR E	3 400	-21.608	55.403	63.336	1.00 72.03	С
MOTA	6079	OG1	THR E	3 400	-21.284	54.169	62.681	1.00 78.00	0
ATOM	6080	CG2	THR E	3 400	-22.412	56.297	62.406	1.00 71.81	С
					-19.443	54.325	65.169	1.00 75.75	N
ATOM	6081	N		3 401					
ATOM	6082	CA		3 401	-19.037	53.592	66.370	1.00 71.37	С
ATOM	6083	С	SER E	3 401	-18.803	54.403	67.649	1.00 64.98	С
ATOM	6084	0	SER E	3 401	-18.296	55.530	67.605	1.00 66.87	0
ATOM	6085	ĊВ	SER I		-17.783	52.763	66.064	1.00 79.12	С
							65.133	1.00 93.93	ŏ
ATOM	6086	OG.		3 401	-18.066	51.735			
MOTA	6087	N		3 402	-19.185	53.814	68.785	1.00 58.91	N
ATOM	6088	CA	ARG I	3 402	-19.010	54.440	70.097	1.00 60.47	С
ATOM	6089	Ċ		3 402	-18.072	53.555	70.926	1.00 60.73	Ċ
							71.217	1.00 65.99	ō
MOTA	6090	0		3 402	-18.393	52.403			
MOTA	6091	CB		3 402	-20.356	54.571	70.821	1.00 56.93	С
ATOM	6092	CG	ARG I	3 402	-20.735	55.997	71.206	1.00 67.01	С
ATOM	6093	CD	ARG F	3 402	-21.916	56.011	72.174	1.00 79.70	С
	6094			3 402	-22.307	57.362	72.592	1.00 93.49	Ň
MOTA		NE							
MOTA	6095	CZ		3 402	-21.562	58.171	73.345	1.00 97.84	С
ATOM	6096	NH1	ARG 1	3 402	-20.369	57.780	73.777	1.00102.38	N
MOTA	6097	NH2	ARG I	3 402	-22.012	59.375	73.673	1.00100.40	N
ATOM	6098	N		3 403	-16.906	54.083	71.294	1.00 58.80	N
ATOM	6099	CA	LEU I		-15.962	53.308	72.094	1.00 54.80	Č
ATOM	6100	С	LEU I	3 403	-16.064	53.611	73.580	1.00 58.34	С
MOTA	6101	0	LEU I	3 403	-15.994	54.765	74.020	1.00 61.62	0
ATOM	6102	СB		3 403	-14.519	53.527	71.641	1.00 56.95	С
									č
ATOM	6103	CG		3 403	-13.565	52.637	72.445	1.00 59.29	
ATOM	6104	CD1	LEU I	3 403	-14.093	51.221	72.409	1.00 66.38	С
MOTA	6105	CD2	LEU I	3 403	-12.159	52.689	71.894	1.00 60.54	С
MOTA	6106	N		3 404	-16.241	52.543	74.343	1.00 61.81	N
						52.617	75.787	1.00 64.91	Ĉ
ATOM	6107	CA		3 404	-16.368				
MOTA	6108	С		3 404	-15.286	51.789	76.448	1.00 62.09	ç
ATOM	6109	0	ARG I	3 404	-14.918	50.715	75.957	1.00 62.39	0
MOTA	6110	CB		3 404	-17.725	52.077	76.217	1.00 74.76	С
ATOM	6111	ĊĞ		3 404	-17.807	51.740	77.694	1.00 87.75	С
								1.00101.27	č
MOTA	6112	CD		3 404	-19.203	51.278	78.064	_	
ATOM	6113	NE		B 404	-19.326	51.032	79.496	1.00111.43	N
MOTA	6114	CZ	ARG I	3 404	-20.483	50.864	80.125	1.00115.18	С
ATOM	6115		ARG I	3 404	-21.620	50.914	79.442	1.00121.83	N
					-20.504	50.658	81.436	1.00114.89	N
ATOM	6116		ARG I						N
MOTA	6117	N		B 405	-14.790	52.274	77.576	1.00 59.43	
ATOM	6118	CA	SER I	3 405	-13.762	51.544	78.274	1.00 62.10	Ç
ATOM	6119	С	SER I	B 405	-13.633	52.062	79.692	1.00 57.60	С
ATOM	6120	ō		3 405	-13.913	53.223	79.965	1.00 63.06	0
ATOM				3 405 3 405	-12.436	51.691	77.531	1.00 66.47	č
	6121	CB							ŏ
ATOM	6122	OG		3 405	-11.509	50.688	77.932	1.00 72.72	
MOTA	6123	N		3 406	-13.209	51.182	80.591	1.00 49.38	N
MOTA	6124	CA		3 406	-13.027	51.536	81.983	1.00 43.52	С
ATOM	6125	c		3 406	-11.541	51.839	82.226	1.00 41.81	С
				3 406	-10.659	51.210	81.632	1.00 42.20	ŏ
ATOM	6126	0							Č
MOTA	6127	CB		3 406	-13.485	50.386	82.879	1.00 48.35	
ATOM	6128	CG		3 406	-14.881	49.923	82.604	1.00 53.45	С
ATOM	6129		HIS I		-15.880	49.957	83.552	1.00 62.61	N
	- 6130						-81-488-	-1-00-60-64-	
ATOM			HIS		-16.996	49.478	83.033	1.00 64.26	č
	6131								
ATOM	6132		HIS		-16.756	49.134	81.782	1.00 67.22	N
MOTA	6133	N		B 407	-11.263	52.797	83.104	1.00 39.08	N
ATOM	6134	CA	ILE I	B 407	-9.888	53.193	83.419	1.00 41.63	С
ATOM	6135	c		B 407	-9.629	53.263	84.934	1.00 43.98	Ċ
ATOM	6136	ŏ		B 407	-10.368	53.929	85.665	1.00 56.43	ŏ
ATOM	6137	CB		B 407	-9.602	54.568	82.817	1.00 35.57	c
			TIP	B 407	-9.846	54.533	81.314	1.00 21.75	С
ATOM	6138	CG1	ILL	3 407					
	6138 6139		ILE		-8.179	55.007	83.148	1.00 38.47	Ċ
MOTA MOTA	6139	CG2	ILE :	B 407	-8.179	55.007	83.148	1.00 38.47	С
ATOM ATOM ATOM	6139 6140	CG2	ILE :	B 407 B 407	-8.179 -10.134	55.007 55.875	83.148 80.751	1.00 38.47 1.00 19.17	C C
ATOM ATOM ATOM ATOM	6139 6140 6141	CG2 CD1 N	ILE I	B 407 B 407 B 408	-8.179 -10.134 -8.573	55.007 55.875 52.591	83.148 80.751 85.396	1.00 38.47 1.00 19.17 1.00 36.98	С С N
ATOM ATOM ATOM	6139 6140	CG2	ILE I	B 407 B 407	-8.179 -10.134	55.007 55.875	83.148 80.751	1.00 38.47 1.00 19.17	C C

ATOM	6143	С	ASN	R	408	-7.75	ξQ	53.942	87.340	1.00 1	7 60	С
	6144	ŏ	ASN		408	-7.22						ŏ
MOTA		_						54.753	86.579	1.00	3.31	
MOTA	6145	CB	ASN		408	-7.14		51.535	87.143	1.00 2		c
MOTA	6146	ÇG	ASN		408	-7.57		50.097	86.840	1.00 3	2.06	Ç
ATOM	6147	OD1	ASN	В	408	-8.75	55	49.756	86.900	1.00 4	5.34	0
MOTA	6148	ND2	ASN	В	408	-6.60)1	49.243	86.543	1.00 2	9.00	N
MOTA	6149	N	PRO		409	-7.94		54.206	88.638	1.00 1		N
	6150	CA	PRO			-7.52		55.477	89.225	1.00 2		Ċ
MOTA												Č
MOTA	6151	C	PRO		409	-6.03		55.712	88.995	1.00 2		Ċ
MOTA	6152	0	PRO		409	-5.22		54.817	89.236	1.00 2		0
ATOM	6153	CB	PRO	В	409	-7.87	70	55.303	90.714	1.00 2	7.72	С
ATOM	6154	CG	PRO	В	409	-9.10)9	54.488	90.668	1.00 1	9.87	С
ATOM	6155	CD	PRO		409	-8.75		53.431	89.595	1.00 1		С
	6156	N	THR		410					1.00 2		N
MOTA						-5.68		56.917	88.542			
MOTA	6157	CA	THR		410	-4.29		57.314	88.274	1.00 2		C
MOTA	6158	С	THR	В	410	-3.67	70	56.447	87.192	1.00 1		С
MOTA	6159	0	THR	В	410	-2.48	33	56.569	86.894	1.00 2	0.31	0
MOTA	6160	CB	THR	В	410	-3.39	90	57.249	89.550	1.00 2	2.26	С
ATOM	6161	OG1	THR		410	-2.83		55.936	89.705	1.00 2	5.09	0
ATOM	6162		THR		410	-4.19		57.590	90.795		6.29	Ċ
					411			55.568		1.00	9.30	N
MOTA	6163	N	GLY			-4.47			86.604			
ATOM	6164	CA	GLY		411	-3.98		54.698	85.548	1.00 1		c
MOTA	6165	С	GLY		411	-4.22		55.287	84.159	1.00 2		Ç
ATOM	6166	0	GLY	В	411	-4.68	39	56.431	84.038	1.00 2	3.53	0
MOTA	6167	N	THR	В	412	-3.92	27	54.505	83.114	1.00 2	6.18	N
MOTA	6168	CA	THR	В	412	-4.09	86	54.954	81.735	1.00 2	5.29	С
ATOM	6169	C	THR			-4.34		53.803	80.769	1.00 2		С
	6170	ō	THR		412	-3.69		52.764	80.874	1.00 2		ŏ
ATOM												
MOTA	6171	CB	THR		412	-2.84		55.702	81.244	1.00 1		C
MOTA	6172		THR			-2.48		56.709	82 196	1.00 1		0
MOTA	6173	CG2	THR	В	412	-3.10	98	56.351	79.892	1.00 2		С
MOTA	6174	N	VAL	В	413	-5.28	30	53.986	79.838	1.00 2	6.41	N
ATOM	6175	CA	VAL			-5.56		52.970	78.822	1.00 2	1.92	С
MOTA	6176	C	VAL			-5.08		53.513	77.495	1.00 2		С
ATOM	6177	ō	VAL			-5.62		54.495	76.985	1.00 2		Ō
ATOM	6178	СВ	VAL			-7.06		52.669	78.687	1.00 2		č
						-7.29		51.808	77.455	1.00	8.29	č
ATOM	6179		VAL							1.00 2		č
ATOM	6180		VAL			-7.56		51.969	79.942			
MOTA	6181	N	LEU			-4.06		52.871	76.948	1.00 2		N
MOTA	6182	CA	LEU			-3.46		53.271	75.680	1.00 2		Ç
MOTA	6183	С	LEU	В	414	-4.05	54	52.477	74.534	1.00 1		С
ATOM	6184	0	LEU	В	414	-4.06	57	51.247	74.567	1.00 2	21.81	0
MOTA	6185	CB	LEU	В	414	-1.96	55	53.043	75.728	1.00 2	26.69	С
ATOM	6186	CG	LEU	В	414	-1.21	17	53.357	74.449	1.00 2	23.20	С
ATOM	6187		LEU		414	-1.50		54.788	74.061	1.00 1	8.54	C
ATOM	6188		LEU			0.26		53.126	74.666	1.00 2		С
ATOM	6189	N	LEU			-4.5		53.189	73.522	1.00 1		N
						-5.17		52.557	72.355	1.00 2		ċ
ATOM	6190	CA	LEU							1.00 2		č
ATOM	6191	C	LEU			-4.4		52.913	71.083			
MOTA	6192	0	LEU			-3.78		53.961	70.989	1.00 3		0
ATOM	6193	CB	LEU			-6.50		52.993	72.210	1.00 2		Ç
ATOM	6194	CG	LEU	В	415	-7.47	70	52.509	73.323	1.00 3	31.67	С
ATOM	6195	CD1	LEU	В	415	-8.83	31	53.093	73.117	1.00 3	36.91	С
MOTA	6196	CD2	LEU	В	415	-7.52	24	50.999	73.309	1.00 3	31.07	c
ATOM	6197	N	GLN	R	416	-4.52	24	52.034	70.098	1.00 2	23.81	N
ATOM	6198	CA	GLN			-3.93		52.272	68.787	1.00 3		С
MOTA	6199	Č	GLN			-4.96		51.970	67.718	1.00 3		Ċ
ATOM	6200	ŏ	GLN			-5.4		50.852	67.633	1.00 4		ō
	6201	СВ	GLN			-2.72		51.392	68.568	1.00 3		č
ATOM						-2.1		51.548	67.203	1.00 4		č
ATOM	6202	CG	GLN									č
ATOM	6203	CD	GLN			-0.97		50.645	66.985	1.00 6	3.00	
MOTA	6204		GLN			0.08		50.834	67.590	1.00 7		0
MOTA	6205	NE2	GLN	В	416	-1.19		49.631	66.134	1.00 7		N
ATOM	6206	N	LEU	В	417	-5.29	50	52.976	66.901	1.00 3		N
ATOM	6207	CA	LEU	В	417	-6.2	30	52.845	65.833	1.00 4	11.44	С
ATOM	6208	С	LEU			-5.59	94	52.788	64.461	1.00 5	3.96	С
ATOM	6209	ō	LEU			-4.74		53.598	64.117	1.00 5		0
ATOM	6210	ĊВ	LEU			-7.20		54.022	65.860	1.00 2		С
ATOM	6211	CG	LEU			-8.0		54.223	67.120	1.00 1		С
ATOM	6212		LEU			-7.1		54.382	68.370	1.00 2		č
						-8.8		55.455	66.908	1.00 1		č
ATOM	6213		LEU					51.810	63.674	1.00 6		N
ATOM	6214	N	GLU			-5.98						C
ATOM	6215	CA	GLU			-5.45		51.767	62.348	1.00 7		, .
ATOM	6216	Č	GLU			-6.6		51.917	61.447	1.00 7		c
ATOM	6217	0	GLU			-7.7		51.539	61.808	1.00 7		0
ATOM	6218	CB	GLU			-4.7		50.468	62.085	1.00 7		C
MOTA	6219	CG	GLU			-3.69		50.630	60.993	1.00 9		c
ATOM	6220	CD	GLU			-2.5		49.711	61.182	1.0010		c
MOTA	6221		GLU			-2.7		48.476	61.225	1.0011		0
MOTA	6222	OE2	GLU	В	418	-1.3		50.223	61.269	1.0011		0
MOTA	6223	N			419	-6.4	46	52.498	60.279	1.00	76.36	N

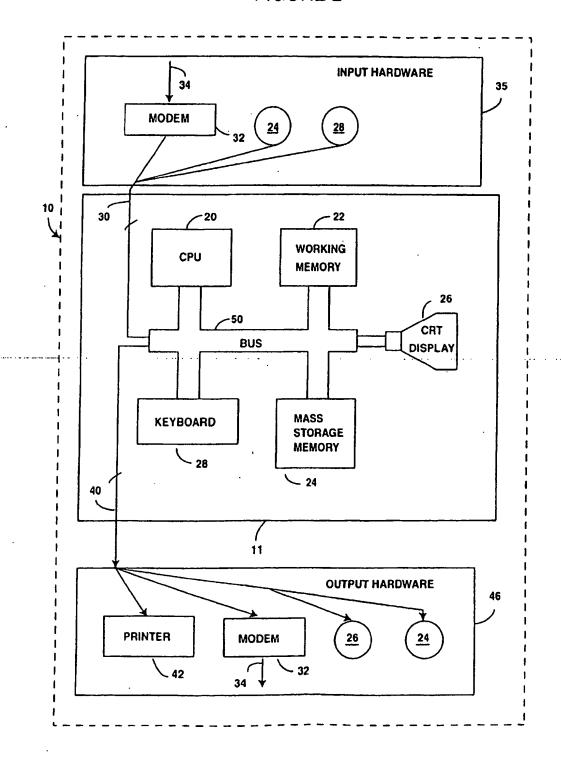
	HETATM	6301	C4	NAG D	693	-17.268	44 337	131.492	1.00101	00	С
				NAG D							
	HETATM		C5			-18.298		130.357	1.00103		С
	HETATM	6303	C6	NAG D	693	-18.792	43.169	129.810	1.00113	. 86	С
	HETATM	6304	C7	NAG D	693	-18.788	48.418	133.800	1.00 79	. 96	С
	HETATM	6305	C8	NAG D		-18.348		134.293	1.00 84		Ċ
	HETATM		N2	NAG D		-17.917		133.052	1.00 74		N
	HETATM	6307	03	NAG D	693 ·	-16.096	45.518	133.268	1.00 68	.40	0
	HETATM	6308	04	NAG D	693	-16.069		130.948	1.00125		ō
	HETATM	6309	Ο5	NAG D		-19.460	45.196	130.824	1.00 83	. 65	0
	HETATM	6310	06	NAG D	693	-17.872	42.123	130.080	1.00132	.47	0
	HETATM	6311	07	NAG D	693	-19.902	47 990	134.095	1.00 69		0
	HETATM		C1	MAN D		-15.378		131.757	1.00140		С
	HETATM	6313	C2	MAN D	694	-14.749	41.758	130.880	1.00146	.70	Ç
	HETATM	6314	C3	MAN D	694	-13.858	40.839	131.720	1.00151	60	С
	-		C4	MAN D		-12.833		132.472			č
	HETATM								1.00151		Ľ.
	HETATM	6316	C5	MAN D	694	-13.537	42.798	133.296	1.00151	.15	C
	HETATM	6317	C6	MAN D	694	-12.576	43.755	133.981	1.00159	.97	Ç
	HETATM		02	MAN D	694	-13.992		129.829	1.00145		ō
	HETATM		03	MAN D		-13.189		130.891	1.00156		0
	HETATM	6320	04	MAN D	694	-12.068	40.865	133.333	1.00152	.15	0
	HETATM	6321	05	MAN D	694	-14.358	43.607	132.435	1.00142	39	0
	HETATM		06	MAN D		-11.225		133.559	1.00177		ō
	HETATM	6323	C1	MAN D	695	-10.712	44.461	132.700	1.00187	. 11	С
	HETATM	6324	C2	MAN D	695	-10.548	43.889	131.286	1.00193	. 26	С
	HETATM		C3	MAN D		-9.530		131.302	1.00195		Č
											×
	HETATM		C4	MAN D		-8.207		131.937	1.00194		C
	HETATM	6327	C5	MAN D		-8.433	43.909	133.278	1.00190	.45	С
	HETATM	6328	C6	MAN D	695	-7.185	44.609	133.750	1.00188	.51	С
	HETATM		02	MAN D		-10.092		130.416	1.00198		ŏ
	HETATM	6330	03	MAN D	695	-9.291		129.973	1.00198	. 31	0
	HETATM	6331	04	MAN D	695	-7.387	42.058	132.152	1.00194	. 30	0
	HETATM		05	MAN D		-9.447		133.148	1.00188		0
						-7.047					
	HETATM		06	MAN D				133.118	1.00184		0
	HETATM	6334	C1	MAN D	696	-13.765	38.597	130.905	1.00160	. 20	С
	HETATM	6335	C2	MAN D	696	-12.677	37.513	131.050	1.00162	.12	С
	HETATM		C3	MAN D		-11.913		129.740	1.00161		C
											Č
	HETATM		C4	MAN D		-12.888		128.611	1.00159		С
	HETATM	6338	C5	MAN D	696	-13.914	38.170	128.510	1.00158	. 37	С
	HETATM	6339	C6	MAN D	696	-14.969	37.903	127.452	1.00154	. 56	С
	HETATM		02	MAN D		-13.303		131.399	1.00165		Õ
	HETATM		03	MAN D		-10.987		129.885	1.00161		0
	HETATM	6342	04	MAN D	696	-12.184	36.909	127.386	1.00155	.90	0
	HETATM	6343	05	MAN D	696	-14.606	38 341	129.770	1.00160	32	0
	HETATM		06	MAN D		-15.435		127.516	1.00146		0
	HETATM	6345	C1	NAG E	715	-13.182	66.020	129.888	1.00120	. 37	С
	HETATM	6346	C2	NAG E	715	-12.899	67.060	130.965	1.00123	.71	С
	НЕТАТМ		C3		715	-12.596		132.294	1.00133		C
											Š
	HETATM		C4	NAG E	715	-13.650		132.649	1.00139		C
	HETATM	6349	C5	NAG E	715	-13.975	64.405	131.442	1.00137	. 63	С
	HETATM	6350	C6	NAG E	715	-15.186	63.543	131.714	1.00140	.83	C
	HETATM		C7	NAG E	715	-11.829		130.601	1.00109		С
						-10.593		130.149	1.00108		č
	HETATM		C8	NAG E	715						
	HETATM	6353	N2	NAG E	715	-11.766	67.865	130.552	1.00113	.83	N
	HETATM	6354	03	NAG E	715	-12.541	67.322	133.330	1.00132	.54	0
	HETATM		04	NAG E	715	-13.185		133.758	1.00146		0
								130.280			ŏ
	HETATM		05	NAG E	715	-14.285			1.00127		
	HETATM		06	NAG E	715	-16.119	64.223	132.547	1.00146		0
	HETATM	6358	07	NAG E	715	-12.822	69.803	130.991	1.00107	.45	0
	HETATM	6359	C1	NAG E	716	-14.007	64.457	134.873	1.00153	. 38	С
	HETATM		C2	NAG E		-13.371		135.988	1.00156		č
	HETATM		C3	NAG E		-14.210		137.263	1.00160		C
	HETATM	6362	C4	NAG E	716	-14.435	65.147	137.669	1.00163	. 56	С
	HETATM	6363	C5	NAG E	716	-15.038	65.907	136.472	1.00158	. 89	С
	HETATM		C6	NAG E		-15.260		136.718	1.00156		Č
	HETATM		C7	NAG E		-12.189		134.965	1.00152		C
	HETATM	6366	C8	NAG E	716	-12.169		134.580	1.00150	. 30	С
	HETATM	6367	N2	NAG E	716	-13.278	62.212	135.582	1.00154	.14	N
	HETATM		03	NAG E		-13.568		138.314	1.00162		0
											ŏ
	HETATM		04	NAG E		-15.317		138.816	1.00173		
	HETATM		05	NAG E		-14.168		135.320	1.00155		0
	HETATM	6371	06	NAG E	716	-16.102	67.940	135.721	1.00150	. 07	0
	HETATM		07	NAG E		-11.235		134.683	1.00152		0
	HETATM		ci	MAN E				140.058	1.00179		č
						-14.704					~
	HETATM		C2	MAN E		-15.550		140.967	1.00179		C
	HETATM	6375	C3	man e		-14.922		142.375	1.00179		Č
1	HETATM	6376	C4	MAN E	717	-14.602	65.041	142.953	1.00181		С
	HETATM		C5	MAN E		-13.811		141.935	1.00181		č
								142.404			c
	HETATM		C6	MAN E		-13.514			1.00176		
	HETATM		02	MAN E		-16.895		141.057	1.00178		0
	HETATM	6380	03	MAN E	717	-15.793	67.148	143.255	1.00174	.10	0
	HETATM		04	MAN E		-13.845		144.149	1.00184		ŏ
					-				•		_

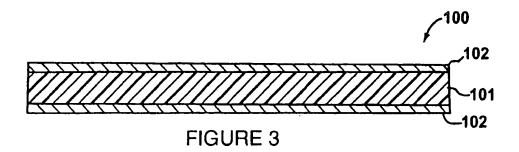
HETATM	6382	05	MAN E 717	-14.530	64 100	140.676	1.00182.95	0
HETATM		06	MAN E 71			141.331	1.00170.00	0
HETATM	6384	C1	NAG F 639	32.119	83.029	85.947	1.00126.87	С
HETATM	6385	C2	NAG F 639	31.123	83.873	85.146	1.00132.58	Ċ
								Č
HETATM	6386	C3	NAG F 639			84.522	1.00142.72	. с
HETATM	6387	C4	NAG F 639	32.640	85.843	85.573	1.00144.73	· c
HETATM		C5				86.479		ž
			NAG F 639				1.00141:68	С
HETATM	6389	C6	NAG F 639	33.956	85.709	87.677	1.00145.51	С
HETATM		C7	NAG F 639			83.912	1.00114.73	č
								Č
HETATM	6331	C8	NAG F 639			82.789	1.00113.10	C
HETATM	6392	N2	NAG F 639	30.525	83.075	84.096	1.00122.92	N
		03	NAG F 639			83.937	1.00153.03	
HETATM								0
HETATM	6394	04	NAG F 639	33.530	86.765	84.919	1.00152.34	0
HETATM	6395	05	NAG F 639	32.688	83.834	86.990	1.00133.39	0
HETATM							1.00154.44	
		06	NAG F 639			87.906		0
HETATM	6397	07	NAG F 639	28.449	83.760	84.617	1.00103.75	0
HETATM	6398	C1	NAG F 640	33.137	88.089	84.918	1.00160.26	Ċ
								_
HETATM		C2	NAG F 640			84.918	1.00165.79	С
HETATM	6400	C3	NAG F 640	33.874	90.433	84.975	1.00166.89	С
HETATM	6401	C4	NAG F 640			83.827	1.00166.57	Ċ
								Č
HETATM	6402	C5	NAG F 640	31.829	89.650	83.659	1.00162.73	Ċ
HETATM	6403	C6	NAG F 640	31.206	89.777	82.285	1.00163.21	Ċ
HETATM		C7	NAG F 640			85.907	1.00168.89	Č
								_
HETATM	6405	C8	NAG F 640	37.313	88.220	87.164	1.00167.41	С
HETATM	6406	N2	NAG F 640	35.201	88.697	86.063	1.00169.98	N
HETATM		03	NAG F 640			84.909	1.00166.81	Ō
HETATM	6408	04	NAG F 640	32.271	91.975	84.072	1.00172.21	0
HETATM		05	NAG F 640			83.730	1.00159.82	ō
HETATM		06	NAG F 640			81.279	1.00163.84	0
HETATM	6411	07	NAG F 640	37.070	88.569	84.812	1.00166.29	0
HETATM		C1	MAN F 641			83.167	1.00180.23	Ċ
								_
HETATM		C2	MAN F 641			83.144	1.00181.77	С
HETATM	6414	C3	MAN F 641	31.609	95.378	82.683	1.00183.44	Ċ
HETATM	6415	C4	MAN F 641			82.878	1.00185.67	Ċ
								_
HETATM		C5	MAN F 641	34.077		82.765	1.00188.14	С
HETATM	6417	C6	MAN F 641	35.503	95.137	83.126	1.00190.39	С
HETATM	6418	02	MAN F 641			84.446	1.00182.75	Ó
HETATM	6419	03	MAN F 641	30.773	96.214	83.495	1.00186.38	0
HETATM	6420	04	MAN F 641	33.357	96.858	81.921	1.00182.05	0
HETATM		05	MAN F 641			83.648	1.00185.32	ō
HETATM	6422	06	MAN F 641	36.496	94.413	82.345	1.00194.64	0
HETATM	6423	C1	MAN F 642	29.936	97.176	82.914	1.00189.51	C
HETATM		C2	MAN F 642			82.097	1.00190.77	ċ
								Č
HETATM	6425	C3	MAN F 642	31.732	98.953	83.014	1.00193.36	C
HETATM	6426	C4	MAN F 642	31.007	99.548	84.231	1.00196.45	С
		C5						č
HETATM			MAN F 642			84.910	1.00197.04	
HETATM	6428	C6	MAN F 642	29.298	98.985	86.072	1.00198.31	С
HETATM	6429	02	MAN F 642	29.917	99.076	81.421	1.00189.27	0
HETATM		03	MAN F 642			82.278	1.00193.29	ō
HETATM	6431	04	MAN F 642			85.159	1.00198.31	0
HETATM	6432	05	MAN F 642	29.244	97.892	83.935	1.00193.89	0
HETATM		06	MAN F 642			86.145	1.00198.31	Ó
HETATM	6434	C1	MAN F 643	35.990	93.378	81.534	1.00198.31	С
HETATM	6435	C2	MAN F 643	36.782	92.081	81.772	1.00198.31	C
HETATM		C3	MAN F 643			81.187	1.00198.31	Č
								č
HETATM		C4	MAN F 643	38.117	92.592	79.710	1.00197.82	Č
HETATM	6438	C5	MAN F 643	37.307	93.883	79.557	1.00196.82	С
HETATM	6439	C6	MAN F 643	37.111	94.291	78.111	1.00194.00	С
		02						ŏ
HETATM			MAN F 643	36.100		81.162	1.00198.31	_
HETATM	6441	03	MAN F 643	38.872		81.327	1.00196.63	0
HETATM	6442	04	MAN F 643	39.427		79.206	1.00194.91	0
HETATM		05	MAN F 643			80.139	1.00198.31	ō
HETATM		06	MAN F 643	35.953		77.550	1.00188.74	0
HETATM	6445	C1	FUC F 644	32.433	86.921	89.162	1.00159.25	С
HETATM		C2	FUC F 644	33.063		90.188	1.00160.27	
								с с
HETATM		C3	FUC F 644	34.526		90.381	1.00161.26	C
HETATM	6448	C4	FUC F 644	34.602	87.805	90.850	1.00162.65	С
HETATM		C5	FUC F 644	33.873		89.841	1.00161.15	č
								_
HETATM		C6	FUC F 644	33.817		90.238	1.00159.96	ç
HETATM	6451	02	FUC F 644	32.956	84.618	89.743	1.00160.19	0
HETATM		03	FUC F 644	35.136		91.330	1.00161.08	ō
HETATM		04	FUC F 644	33.975		92.120	1.00166.93	Ō
HETATM	6454	05	FUC F 644	32.513	88.244	89.671	1.00159.60	0
HETATM		Cl	NAG G 692			61.043	1.00 81.28	С
HETATM			NAG G 692			60.977		č
		C2					1.00 89.99	C
HETATM		C3	NAG G 692		67.603	59.625	1.00 91.14	С
HETATM	6458	C4	NAG G 692			59.204	1.00 89.04	c
HETATM			NAG G 692			59.186		ž
		C5					1.00 83.33	c c
HETATM		C6	NAG G 692			58.666	1.00 86.45	С
HETATM	6461	C7	NAG G 692	29.018	67.014	62.319	1.00101.90	С
HETATM		C8	NAG G 692			62.450		č
	3404	CO	14AG G 092	30.453	00.330	02.450	1.00102.83	·

HETATM	6463	N2	NAG G	692	28.695	67.645	61.192	1.00 97.33	N
HETATM		03	NAG G		26.613	66.201	59.704	1.00 94.88	0
HETATM		04	NAG G		25.126	67.837	57.887	1.00 95.09	0
HETATM HETATM		05 06	NAG G		26.146 23.430	70.251 70.092	60.521 58.975	1.00 73.85	0
HETATM		07	NAG G		28.219	66.809	63.233	1.00 86.10 1.00101.45	ŏ
HETATM		C1	NAG G		23.871	67.233	57.756	1.00 98.64	С
HETATM		C2	NAG G		23.321	67.464	56.335	1.00 95.54	С
HETATM		C3	NAG G		21.965	66.769	56.169	1.00 98.16	C
HETATM HETATM		C4 C5	NAG G NAG G		22.030 22.757	65.297 65.103	56.580 57.934	1.00105.51 1.00108.87	C
HETATM		C6	NAG G		23.069	63.640	58.214	1.00103.67	Ċ
HETATM		c7	NAG G		24.226	69.586	55.632	1.00 93.26	С
HETATM		C8	NAG G		24.005	71.065	55.377	1.00 87.73	Ċ
HETATM		N2	NAG G		23.183	68.884	56.070	1.00 91.40	N
HETATM HETATM		03 04	NAG G		21.548	66.851 64.776	54.818 56.677	1.00 87.79 1.00114.16	0
HETATM		05	NAG G		24.024	65.819	57.970	1.00102.56	ŏ
HETATM		06	NAG G	693	22.449	62.779	57.263	1.00119.18	0
HETATM		07	NAG G		25.340	69.094	55.434	1.00101.16	0
HETATM		C1 C2	MAN G		20.286	63.958	55.639 56.066	1.00119.37	C
HETATM HETATM		C3	MAN G		19.098 18.780	63.069 62.208	54.854	1.00121.53	0000
HETATM		C4	MAN G		18.409	63.081	53.662	1.00129.09	č
HETATM	6487	C5	MAN G		19.574	64.023	53.357	1.00130.74	С
HETATM		C6	MAN G		19.188	64.996	52.274	1.00141.14	c
HETATM		02	MAN G		17.976 17.763	63.876 61.211	56.409 55.108	1.00125.53 1.00113.48	0
HETATM HETATM		03 04	MAN G		18.152	62.263	52.530	1.00136.46	ő
HETATM		05	MAN G		19.915	64.791	54.532	1.00121.09	ŏ
HETATM	6493	06	MAN G	694	20.318	65.793	51.893	1.00154.48	0
HETATM		C1	MAN G		17.828	60.147	54.190	1.00113.74	c
HETATM		C2	MAN G		17.347	58.835 58.337	54.818 55.863	1.00111.77	00000
HETATM HETATM		C3 C4	MAN G		18.355 19.766	58.266	55.265	1.00117.80	č
HETATM		C5	MAN G		20.118	59.626	54.673	1.00117.97	Č
MTATAH	6499	C6	MAN G		21.498	59.749	54.057	1.00117.01	C
HETATM		02	MAN G		17.217	57.856	53.796	1.00 96.60	0
HETATM		03	MAN G		17.970 20.700	57.052 57.925	56.331 56.277	1.00120.40	0 0
HETATM HETATM		04 05	MAN G		19.144	59.971	53.668	1.00120.33	ŏ
HETATM		06	MAN G		21.834	58.594	53.308	1.00113.39	0
HETATM	6505	C1	MAN G		19.885	66.898	51.143	1.00164.32	0000
HETATM		C2	MAN G		21.062	67.519	50.365	1.00166.62	C
HETATM HETATM		C3	MAN G		22.001	68.326 69.232	51.285 52.282	1.00171.12	6
HETATM		C4 C5	MAN G		20.073	68.476	52.948	1.00173.34	č
HETATM		C6	MAN G		19.196	69.358	53.827	1.00172.72	C
HETATM		02	MAN G		20.585	68.356	49.314	1.00163.60	0
HETATM		03		696	22.877	69.128	50.491	1.00169.59	0
HETATM HETATM		04 05	MAN G		22.124 19.229	69.702 67.884	53.294 51.939	1.00179.94	ő
HETATM		06	MAN G		19.108	70.684	53.320	1.00172.71	0
HETATM		C1	NAG H	715	13.640	83.037	66.153	1.00115.84	C
HETATM		C2	NAG H		12.944	84.348	65.800	1.00117.74	C
HETATM		C3		715 715	12.827 14.059	84.533 84.079	64.279 63.468	1.00130.57 1.00140.47	,
HETATM HETATM		C4 C5	NAG H	715	14.747	82.839	64.066	1.00137.92	C
HETATM		C6	NAG H		16.121	82.604	63.466	1.00140.32	С
HETATM		C7	NAG H		11.226		67.210	1.00 95.61	Č
HETATM		C8	NAG H		9.809	85.192	67.743	1.00 87.49	C N
HETATM HETATM		N2 03		715 715	11.611 12.579	84.340 85.904	66.371 63.987	1.00105.35	Ö
HETATM		04		715	13.614	83.755	62.132	1.00155.63	ŏ
HETATM	6527	05		715	14.904	82.978	65.491	1.00126.15	0
HETATM		06		715	17.064	82.210	64.447	1.00143.48	0
HETATM		07	NAG H		11.952 14.154	86.224 84.450	67.555 61.069	1.00 91.56 1.00170.24	0 C
HETATM HETATM		C1 C2		716 716	14.134	83.462	59.946	1.00178.62	С
HETATM		C3		716	14.948	84.201	58.720	1.00182.32	С
HETATM	6533	C4	NAG H	716	13.979	85.302	58.305	1.00182.82	С
HETATM		C5		716	13.630	86.201	59.513 59.199	1.00181.47	c c
HETATM HETATM		C6 C7		716 716	12.531 15.013	87.178 81.194	60.478	1.00183.71	С
HETATM		c8		716	16.059	80.205	60.959	1.00184.71	С
HETATM	6538	N2	NAG H	716	15.382	82.468	60.395	1.00181.87	N
HETATM		03	NAG H		15.138	83.291	57.652	1.00185.53	0
HETATM HETATM		04 05	NAG H		14.571 13.181	86.094 85.413	57.256 60.646	1.00183.84	0
HETATM		06	NAG H		12.397	88.161	60.216	1.00172.00	ŏ
НЕТАТМ		07	NAG H		13.881	80.804	60.195	1.00183.38	0

```
MAN H 717
HETATM 6544
              C1
                                    13.820
                                             86.274
                                                      56.101
                                                               1.00184.69
HETATM 6545
              C2
                   MAN H 717
                                    13.250
                                             87.719
                                                      56.059
                                                               1.00183.61
HETATM 6546
               C3
                   MAN H 717
                                    12.670
                                              88.105
                                                      54.679
                                                               1.00185.94
HETATM 6547
               C4
                   MAN H 717
                                    13.602
                                             87.681
                                                      53.533
                                                               1.00190.00
                   MAN H 717
HETATM 6548
               C5
                                    14.036
                                             86.209
                                                      53.703
                                                               1.00191.21
                   MAN H 717
                                    14.958
HETATM 6549
              C6
                                             85.664
                                                      52.604
                                                               1.00190.18
                          717
                   MAN H
                                    14.249
                                             88.653
                                                               1.00178.99
HETATM 6550
              02
                                                      56,450
              03
                   MAN H 717
                                    12.417
                                                               1.00181.42
HETATM 6551
                                             89.514
                                                      54.633
                   MAN H 717
                                    12.959
                                             87.878
                                                      52.278
                                                               1.00190.59
HETATM 6552
              04
              05
HETATM 6553
                   MAN H 717
                                    14.701
                                             86.037
                                                      54.987
                                                               1.00188.51
              06
                   MAN H 717
                                    14.994
                                             84.241
                                                      52.603
                                                               1.00188.39
HETATM 6554
                                  GALACTOSE MOLECULE COORDINATES
             Atom
            Type Resid
                                   <u>X</u>
-17.781
                                             Y Z
61.062 105.414
HETATM 6555
                         1101
                                                               1.00 61.45
                                                                                        С
                                                                                       000
                                   -16.853
HETATM 6556
              C2
                   GAL
                        1101
                                             59.968 105.952
                                                               1.00 59.70
                                                               1.00 57.27
HETATM 6557
              C3
                   GAL
                         1101
                                   -16.406
                                             59.043 104.831
                                             58.457 104.235
59.590 103.680
HETATM 6558
              C4
                   GAL
                         1101
                                   -17.672
                                                               1.00 55.95
                        1101
                                   -18.524
                                                               1.00 62.81
HETATM 6559
              C5
                   GAL
                                   -19.797
                                             59.114 103.010
HETATM 6560
              C6
                   GAL
                         1101
                                                               1.00 66.98
                         1101
                                   -17.082
                                             61.854 104.525
                                                               1.00 60.34
HETATM 6561
              01
                   GAL
HETATM 6562
              02
                         1101
                                   -15.728
                                             60.529 106.610
                                                               1.00 61.68
                   GAL
                                   -15.549
                                             58.009 105.328
HETATM 6563
               03
                   GAL
                         1101
                                                               1.00 56.11
                                                                                        o
                                   -18.379
                                                               1.00 47.84
HETATM 6564
              04
                   GAL
                         1101
                                             57.776 105.258
                                                                                        0
                                             60.485 104.733
60.192 102.791
                                   -18.909
                                                               1.00 64.69
                         1101
                                                                                        o
HETATM 6565
              05
                   GAL
HETATM 6566
                                   -20.698
                                                               1.00 69.17
                         1101
                                                                                        0
              06
                   GAL
                                    19.728
                                             69.733
                                                      87.085
                                                               1.00 73.14
HETATM 6567
              Cl
                   GAL
                         1103
HETATM 6568
              C2
                         1103
                                    19.032
                                             68.891
                                                      86.002
                                                               1.00 74.89
                   GAL
HETATM 6569
              C3
                   GAL
                         1103
                                    18.997
                                             67.401
                                                      86.351
                                                               1.00 73.18
                                    20.418 21.069
                                             66.932
67.816
                                                               1.00 67.98
HETATM 6570
              C4
                   GAL
                         1103
                                                      86.650
                                                      87.740
HETATM 6571
              C5
                   GAL
                         1103
                                    22.533
                                             67.422
                                                      87.991
                                                               1.00 68.59
HETATM 6572
              C6
                   GAL
                         1103
                                    18.964
                                             69.722
HETATM 6573
              01
                         1103
                                                      88.243
                                                               1.00 64.62
                   GAL
                                    17.708
                                             69.354
                                                      85.806
                                                               1.00 82.04
HETATM 6574
              02
                   GAL
                         1103
HETATM 6575
              03
                   GAL
                         1103
                                    18.444
                                             66.627
                                                      85.276
                                                               1.00 75.70
                                                                                        0
нетатм 6576
              04
                   GAL
                         1103
                                    21.194
                                             66.934
                                                      85.456
                                                               1.00 55.41
                                                                                        o
                                                               1.00 77.47
HETATM 6577
              05
                   GAL
                         1103
                                    21.051
                                             69.220
                                                      87.364
                                                                                        O
HETATM 6578
              06
                  GAL
                         1103
                                    23.045 67.950
                                                     89.214
                                                                                        0
                              ETHYLENE GLYCOL MOLECULE COORDINATES
             Atom
             Type Resid
                        ! <u>#</u>
1102
1102
                                             <u>Y</u> <u>Z</u>
35.815 115.706
34.746 116.032
                                                               OCC B
1.00104.60
1.00102.85
                                    X
21.911
HETATM 6579
                                                                                        c
              C1
                   EGL
                                    21.022
HETATM 6580
                   EGL
              01
                                                                1.00103.58
                                    21.852
                                             36.116 114.185
HETATM 6581
              C2
                   EGL
                         1102
                                             35.242 113.531
39.439 90.310
HETATM 6582
               02
                   EGL
                         1102
                                    20.925
                                                                1.00 95.95
HETATM 6583
              Cl
                   EGL
                         1104
                                    19.899
                                                               1.00108.69
                                    20.931 40.421 90.338
19.324 39.275 91.722
20.002 40.157 92.629
HETATM 6584
              01
                   EGL.
                         1104
                                                               1.00105.85
                                                                                        0
HETATM 6585
              C2
                   EGL.
                         1104
                                                               1.00106.50
                                                                                        C
              02
                                                               1.00103.98
HETATM 6586
                   EGL
                        1104
                                    WATER MOLECULE COORDINATES
             Atom
                           1
             Type Resid
                                     <u>X</u>
4.389
                                             <u>Y</u> <u>Z</u> 62.036 109.896
                                                               OCC B
1.00 36.21
HETATM 6587
             0
                   НОН
HETATM 6588
                            2
                                    -33.743
                                             66.424
                                                      98.001
                                                               1.00 49.95
                   нон
                                   -31.308
                                             61.068
HETATM 6589
                   нон
                                                      97.174
                                                               1.00 14.32
                                             39.358 106.515
HETATM 6590
              0
                   HOH
                            4
                                     7.246
                                                               1.00 49.50
                                                                                        0
                                             56.381 115.242
72.666 75.302
68.845 89.368
                                                               1.00 82.65
HETATM 6591
              O
                   HOH
                            5
                                    -4.342
                                                               1.00 22.68
HETATM 6592
                   нон
              0
                            6
7
                                    -5.596
                                     7.443
HETATM 6593
              0
                   HOH
                                                               1.00 49.14
                   нон
                                   -34.391
                                             44.412 107.214
                                                               1.00 32.63
HETATM 6594
                            8
HETATM 6595
                   HOH
                                   -12.650
                                             42.533 120.345
                                                               1.00 32.46
                                                                                        0
                                             67.495 82.217
56.527 97.931
                                                               1.00 35.71
1.00 36.76
HETATM 6596
              O
                   нон
                           10
                                    -2.388
                   HOH
HETATM 6597
              0
                           11
                                    36.062
                                             49.180 67.281
                                                               1.00 35.06
                   HOH
HETATM 6598
                                    15.246
              0
                           12
HETATM 6599
                   нон
                           13
                                    16.887
                                             52.495
                                                      68.847
                                                               1.00 54.15
              0
HETATM 6600
                   нон
                                             64.968 116.907
                                                               1.00 83.42
                                                                                        0
                           14
                                     8.892
                                                               1.00 3.31
1.00 37.68
HETATM 6601
              o
                   нон
                           15
                                    -6.111
                                             64.210 102.918
                                                                                        0
                                             69.993 67.725
79.004 83.860
HETATM 6602
              ٥
                   HOH
                           16
                                    -4.402
                                                                                        O
                                                               1.00 56.31
HETATM 6603
                   нон
                           17
                                     5.852
              0
                                                      90.834
HETATM 6604
                   нон
                                    32.211
                                             64.353
                                                               1.00
                           18
```

FIGURE 2





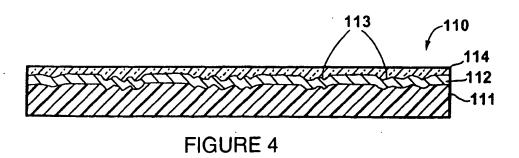


FIGURE 5

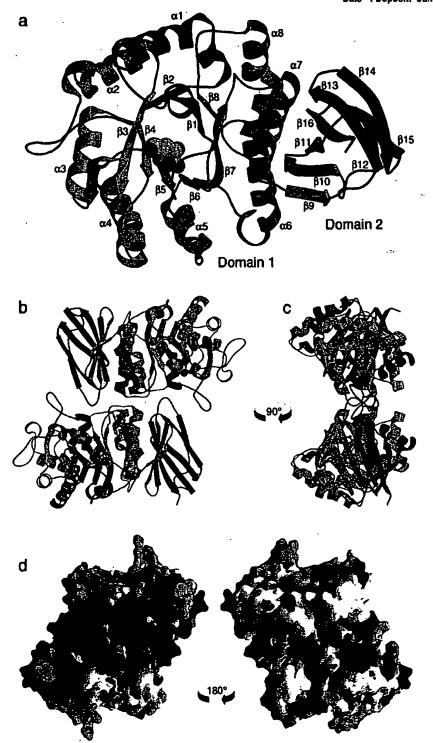


FIGURE 6
BEST AVAILABLE COPY

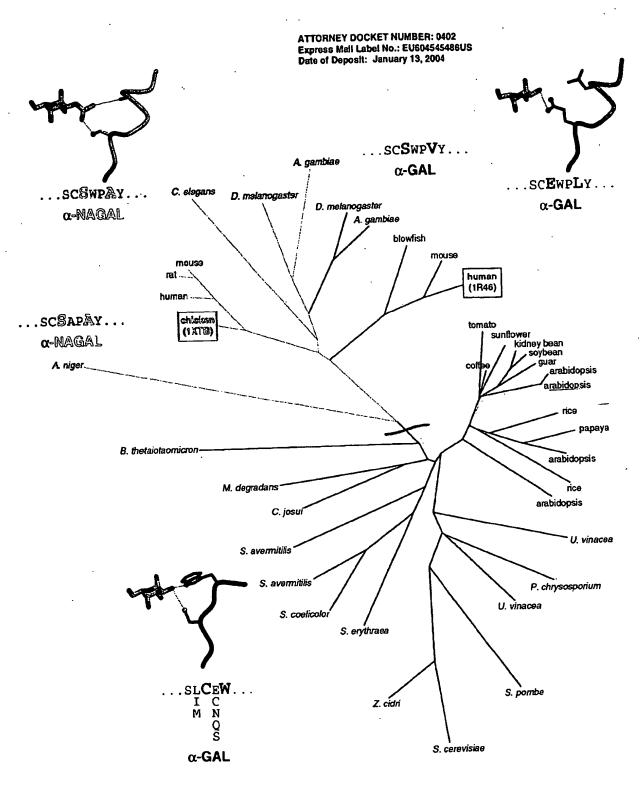


FIGURE 7

ATTORNEY DOCKET NUMBER: 0402 Express Mail Label No.: EU604545486US Date of Deposit: January 13, 2004

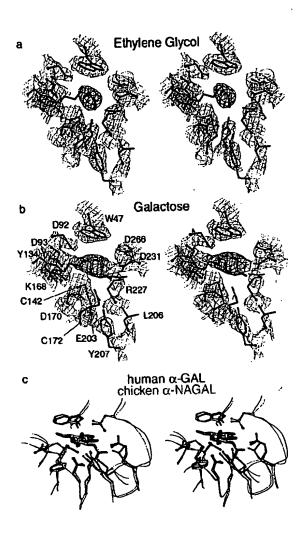
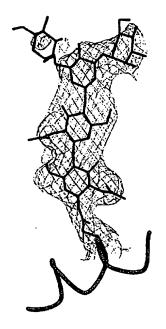


FIGURE 8.

ATTORNEY DOCKET NUMBER: 0402 Express Mail Label No.: EU604545486US Date of Deposit: January 13, 2004

FIGURE 9



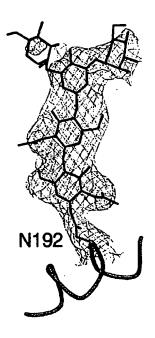


FIGURE 10

APPLICATION DATA SHEET FORM

Inventor Information

Inventor One Given Name::

Family Name::

Postal Address Line One::

City::

State or Province::

Postal or Zip Code:: Citizenship Country::

Inventor Two Given Name::

Family Name::

Postal Address Line One::

City::

State or Province:: Postal or Zip Code::

Citizenship Country::

Inventor Three Given Name::

Family Name::

Postal Address Line One::

City::

State or Province::

Postal or Zip Code::

Citizenship Country::

Inventor Four Given Name::

Family Name::

Postal Address Line One::

City::

State or Province::

Postal or Zip Code::

Citizenship Country::

Inventor Five Given Name::

Family Name::

Postal Address Line One::

City::

State or Province:: Postal or Zip Code::

Citizenship Country::

Inventor Six Given Name::

Family Name::

Postal Address Line One::

612821.1

Scott C.

Garman

Rockville

Maryland 20850

US

David N.

Garboczi

Gaithersburg

Maryland

20877

US

Richard F.

Selden

Wellesley

Massachusetts

02482

US

Douglas A. Treco

Arlington

Massachusetts

02476

US

Michael W.

Heartlein

Boxborough

Massachusetts

01719

US

Marianne

Borowski

Application Data Sheet Form

Page 2

City::

Glen

State or Province::

New Hampshire

Postal or Zip Code::

03838

Citizenship Country::

US

Correspondence Information

Name Line One::

Konstantinos Andrikopoulos, J.D., Ph.D.

Name Line Two::

Address Line One:

Transkaryotic Therapies, Inc.

Address Line Two::

700 Main St.

City::

Cambridge

State or Province::

MA US

Country::

Postal or Zip Code::

02139

Telephone One::

617-613-4255

Telephone Two::

617-349-0200

Fax Number:

617-613-4020

Electronic Mail::

kandrikopoulos@tktx.com

Application Information

Title Line One::

CRYSTAL STRUCTURE OF HUMAN

 α -GALACTOSIDASE

Total Specification Sheets w/Claims::

39

Total Drawing Sheets::

91

Sequence Listing Sheets::

3 8

Claims::

Provisional

Application Type::

0402

Docket Number::

January 13, 2004

Date of deposit::

Express Mail No .::

EU604545486US

Representative Information

Name Line One::

Konstantinos Andrikopoulos, J.D., Ph.D.

Name Line Two::

Address Line One:

Transkaryotic Therapies, Inc.

Address Line Two::

700 Main St.

City::

Cambridge

State or Province::

MA

Country::

US

Postal or Zip Code::

02139

Telephone One::

617-613-4255

Application Data Sheet Form

Page 3

Telephone Two::

617-349-0200

Fax Number:

617-613-4020

Electronic Mail::

kandrikopoulos@tktx.com

Representative Customer Number

Continuity Information

Prior Foreign Applications

Foreign Application One::

Filing Date::

Country::

Priority Claimed::

SEQUENCE LISTING

```
<110> National Institute of Allergy and Infectious Diseases, NIH
       Transkaryotic Therapies, Inc.
       Garman, Scott C.
       Garboczi, David N.
       Selden, Richard F.
       Treco, Douglas A.
       Heartlein, Michael W.
       Borowski, Marianne
<120> CRYSTAL STRUCTURE OF HUMAN ALPHA-GALACTOSIDASE
<130> 0402
<160> 2
<170> PatentIn version 3.2
<210>
      1290
<211>
<212> DNA
<213> Homo sapiens
<400> 1
atgcagctga ggaacccaga actacatctg ggctgcgcgc ttgcgcttcg cttcctggcc
                                                                      60
ctcgtttcct gggacatccc tggggctaga gcactggaca atggattggc aaggacgcct
                                                                     120
accatgggct ggctgcactg ggagcgcttc atgtgcaacc ttgactgcca ggaagagcca
                                                                     180
gatteetgea teagtgagaa getetteatg gagatggeag ageteatggt eteagaagge
                                                                     240
                                                                     300
tggaaggatg caggitatga gtaccictgc attgatgact gitggatggc tccccaaaga
                                                                     360
gattcagaag gcagacttca ggcagaccct cagcgctttc ctcatgggat tcgccagcta
gctaattatg ttcacagcaa aggactgaag ctagggattt atgcagatgt tggaaataaa
                                                                     420
acctgcgcag gcttccctgg gagttttgga tactacgaca ttgatgccca gacctttgct
                                                                     480
                                                                     540
gactggggag tagatctgct aaaatttgat ggttgttact gtgacagttt ggaaaatttg
gcagatggtt ataagcacat gtccttggcc ctgaatagga ctggcagaag cattgtgtac
                                                                     600
tcctgtgagt ggcctcttta tatgtggccc tttcaaaagc ccaattatac agaaatccga
                                                                     660
cagtactgca atcactggcg aaattttgct gacattgatg attcctggaa aagtataaag
                                                                     720
                                                                     780
agtatettgg actggacate ttttaaccag gagagaattg ttgatgttge tggaccaggg
                                                                     840
ggttggaatg acccagatat gttagtgatt ggcaactttg gcctcagctg gaatcagcaa
                                                                     900
gtaactcaga tggccctctg ggctatcatg gctgctcctt tattcatgtc taatgacctc
cgacacatca gccctcaagc caaagctctc cttcaggata aggacgtaat tgccatcaat
                                                                     960
caggacccct tgggcaagca agggtaccag cttagacagg gagacaactt tgaagtgtgg
                                                                    1020
gaacgacctc tctcaggctt agcctgggct gtagctatga taaaccggca ggagattggt
                                                                    1080
ggacctcgct cttataccat cgcagttgct tccctgggta aaggagtggc ctgtaatcct
                                                                    1140
gcctgcttca tcacacagct cctccctgtg aaaaggaagc tagggttcta tgaatggact
                                                                    1200
tcaaggttaa gaagtcacat aaatcccaca ggcactgttt tgcttcagct agaaaataca
                                                                    1260
atgcagatgt cattaaaaga cttactttaa
                                                                    1290
```

<210> 2

<211> 429

<212> PRT

<213> Homo sapiens

Met Gln Leu Arg Asn Pro Glu Leu His Leu Gly Cys Ala Leu Ala Leu 1 $$ 10 $$ 15

Arg Phe Leu Ala Leu Val Ser Trp Asp Ile Pro Gly Ala Arg Ala Leu 20 25 30

Asp Asn Gly Leu Ala Arg Thr Pro Thr Met Gly Trp Leu His Trp Glu 35 40 45

Arg Phe Met Cys Asn Leu Asp Cys Gln Glu Glu Pro Asp Ser Cys Ile 50 60

Ser Glu Lys Leu Phe Met Glu Met Ala Glu Leu Met Val Ser Glu Gly 65 70 75 80

Trp Lys Asp Ala Gly Tyr Glu Tyr Leu Cys Ile Asp Asp Cys Trp Met $85 \hspace{1cm} 90 \hspace{1cm} 95$

Ala Pro Gln Arg Asp Ser Glu Gly Arg Leu Gln Ala Asp Pro Gln Arg 100 105 110

Phe Pro His Gly Ile Arg Gln Leu Ala Asn Tyr Val His Ser Lys Gly 115 120 125

Leu Lys Leu Gly Ile Tyr Ala Asp Val Gly Asn Lys Thr Cys Ala Gly 130 135 140

Phe Pro Gly Ser Phe Gly Tyr Tyr Asp Ile Asp Ala Gln Thr Phe Ala 145 150150155160

Asp Trp Gly Val Asp Leu Leu Lys Phe Asp Gly Cys Tyr Cys Asp Ser 165 170 175

Leu Glu Asn Leu Ala Asp Gly Tyr Lys His Met Ser Leu Ala Leu Asn 180 185 190

Arg Thr Gly Arg Ser Ile Val Tyr Ser Cys Glu Trp Pro Leu Tyr Met 195 200 205

Trp Pro Phe Gln Lys Pro Asn Tyr Thr Glu Ile Arg Gln Tyr Cys Asn 210 $\,$ 215 $\,$ 220 $\,$

His Trp Arg Asn Phe Ala Asp Ile Asp Asp Ser Trp Lys Ser Ile Lys 225 230 240

Ser Ile Leu Asp Trp Thr Ser Phe Asn Gln Glu Arg Ile Val Asp Val 245 250 255

Ala Gly Pro Gly Gly Trp Asn Asp Pro Asp Met Leu Val Ile Gly Asn 260 265 270

Phe Gly Leu Ser Trp Asn Gln Gln Val Thr Gln Met Ala Leu Trp Ala 275 280 285

Ile Met Ala Ala Pro Leu Phe Met Ser Asn Asp Leu Arg His Ile Ser 290 295 300

Pro Gln Ala Lys Ala Leu Leu Gln Asp Lys Asp Val Ile Ala Ile Asn 305 310315315

Gln Asp Pro Leu Gly Lys Gln Gly Tyr Gln Leu Arg Gln Gly Asp Asn 325 330 335

Phe Glu Val Trp Glu Arg Pro Leu Ser Gly Leu Ala Trp Ala Val Ala 340 $$345\$

Met Ile Asn Arg Gln Glu Ile Gly Gly Pro Arg Ser Tyr Thr Ile Ala $355 \hspace{1.5cm} 360 \hspace{1.5cm} 365$

Val Ala Ser Leu Gly Lys Gly Val Ala Cys Asn Pro Ala Cys Phe Ile $370 \hspace{1cm} 375 \hspace{1cm} 380$

Thr Gln Leu Leu Pro Val Lys Arg Lys Leu Gly Phe Tyr Glu Trp Thr 385 390395 400

Ser Arg Leu Arg Ser His Ile Asn Pro Thr Gly Thr Val Leu Leu Gln $405 \hspace{1.5cm} 410 \hspace{1.5cm} 415$

Leu Glu Asn Thr Met Gln Met Ser Leu Lys Asp Leu Leu 420 425